Phenol, 2-(1-methylethyl)-, methylcarbamate

Other names:
2-(1-Methylethyl)-phenol methyl-carbamate
2-(1-Methylethyl)phenyl methylcarbamate
2-Isopropylphenyl N-methylcarbamate
2-Isopropylphenyl methylcarbamate
BAY 105807
BAYER 39731
Bay 39731
Bayer 39,731
Carbamic acid, methyl-, 2-(1-methylethyl)phenyl ester
Carbamic acid, methyl-, o-cumenyl ester
Carbamic acid, methyl-, o-isopropylphenyl ester
ENT 25670
Etrofolan
Hytox
Isoprocarb
Isoprocarbe
Isopropyl phenylmethyl carbamate
Isopropylphenol methylcarbamate
KHE 0145
MIPC
Methylcarbamic acid, o-cumenyl ester
Mipcin
Mipcine
Mipsin
N-Methyl-2-isopropylphenylcarbamate
NSC 191479
O-Cumenyl N-methylcarbamate
OMS 32
PPC 3
Phenol, o-isopropyl-, methylcarbamate
Ro 7-5050
o-Cumenyl methylcarbamate
o-Isopropylphenol methylcarbamate
o-Isopropylphenyl N-methylcarbamate
o-Isopropylphenyl methylcarbamate

Inchi: InChI=1S/C11H15NO2/c1-8(2)9-6-4-5-7-10(9)14-11(13)12-3/h4-8H,1-3H3,(H,12,13)
InchiKey: QBSJMKIUCUGGNG-UHFFFAOYSA-N
Formula: C11H15NO2
SMILES: CNC(=O)Oc1ccccc1C(C)C
Mol. weight [g/mol]: 193.24

CAS: 2631-40-5

Physical Properties

Property code	Value	Unit	Source
gf	-2.45	kJ/mol	Joback Method
hf	-241.92	kJ/mol	Joback Method
hfus	22.26	kJ/mol	Joback Method
hvap	58.22	kJ/mol	Joback Method
log10ws	-2.86		Aqueous Solubility Prediction Method
log10ws	-2.86		Estimated Solubility Method
logp	2.528		Crippen Method
mcvol	159.510	ml/mol	McGowan Method
pc	2796.51	kPa	Joback Method
rinpol	205.40		NIST Webbook
rinpol	1548.00		NIST Webbook
rinpol	1538.00		NIST Webbook
rinpol	1537.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1481.00		NIST Webbook
ripol	2085.00		NIST Webbook
tb	608.76	K	Joback Method
tc	823.24	K	Joback Method
tf	369.94 ± 0.20	K	NIST Webbook
vc	0.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.17	J/mol×K	608.76	Joback Method
cpg	410.54	J/mol×K	644.51	Joback Method
cpg	424.06	J/mol×K	680.25	Joback Method
cpg	436.76	J/mol×K	716.00	Joback Method
cpg	448.64	J/mol×K	751.75	Joback Method
cpg	459.72	J/mol×K	787.50	Joback Method
cpg	470.03	J/mol×K	823.24	Joback Method
hfust	26.14	kJ/mol	369.30	NIST Webbook

hfust	26.14	kJ/mol	369.30	NIST Webbook

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2631405&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume