Fenobucarb

Other names:	(2-butan-2-ylphenyl) N-methylcarbamate
	2-(1-Methylpropyl)phenyl methylcarbamate
	2-sec-Butylphenyl N-methylcarbamate
	2-sec-butylphenyl methylcarbamate
	2-sek.Butylfenylester kyseliny methylkarbaminove
	BAY 41637
	BPMC
	Barizon
	Bassa
	Baycarb
	Bayer 41367C
	Bayer 41637
	Carbamic acid, methyl-, o-sec-butylphenyl ester
	Carvil
	Fenobcarb
	Hopcin
	Methylcarbamic acid o-sec-butylphenyl ester
	Osbac
	Phenol, 2-(1-methylpropyl)-, 1-(N-methylcarbamate)
	Phenol, 2-(1-methylpropyl)-, methylcarbamate
	o-sec-Butylphenyl methylcarbamate
Inchi:	InChI=1S/C12H17NO2/c1-4-9(2)10-7-5-6-8-11(10)15-12(14)13-3/h5-9H,4H2,1-3H3,(H,13
InchiKey:	DIRFUJHNVNOBMY-UHFFFAOYSA-N
Formula:	C12H17NO2
SMILES:	CCC(C)c1ccccc1OC(=O)NC
Mol. weight [g/mol]:	207.27
CAS:	3766-81-2

Physical Properties

Property code	Value	Unit	Source
gf	5.97	kJ/mol	Joback Method
hf	-262.56	kJ/mol	Joback Method
hfus	24.85	kJ/mol	Joback Method
hvap	60.45	kJ/mol	Joback Method
log10ws	-2.53		Aqueous Solubility Prediction Method
logp	2.918		Crippen Method

mcvol	173.600	ml/mol	McGowan Method
pc	2532.82	kPa	Joback Method
rinpol	1618.00		NIST Webbook
rinpol	1570.00		NIST Webbook
rinpol	1609.00		NIST Webbook
rinpol	1567.00		NIST Webbook
rinpol	1608.00		NIST Webbook
rinpol	1608.00		NIST Webbook
rinpol	1621.00		NIST Webbook
rinpol	1567.00		NIST Webbook
rinpol	1612.00		NIST Webbook
rinpol	1621.00		NIST Webbook
rinpol	1617.00		NIST Webbook
rinpol	1609.00		NIST Webbook
rinpol	1608.00		NIST Webbook
rinpol	1570.00		NIST Webbook
rinpol	1562.00		NIST Webbook
ripol	2148.00		NIST Webbook
ripol	2148.00		NIST Webbook
tb	631.64	K	Joback Method
tc	842.61	K	Joback Method
tf	304.65	K	Aqueous Solubility Prediction Method
vc	0.652	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.86	J/mol×K	631.64	Joback Method
cpg	460.85	J/mol×K	666.80	Joback Method
cpg	474.96	J/mol×K	701.96	Joback Method
cpg	488.20	J/mol×K	737.13	Joback Method
cpg	500.60	J/mol×K	772.29	Joback Method
cpg	512.17	J/mol×K	807.45	Joback Method
cpg	522.93	J/mol×K	842.61	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3766812&Units=SI

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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