BAYCARB

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
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

Physical Properties

Property code	Value	Unit	Source
hf	-392.45	kJ/mol	Cheméo Relay (1.0)
hfus	24.85	kJ/mol	Joback Method
hvap	80.83	kJ/mol	Cheméo Relay (1.0)
log10ws	-2.53		Aqueous Solubility Prediction Method
logp	2.918		Crippen Method
mcvol	173.600	ml/mol	McGowan Method
rinpol	1618.00		NIST Webbook
rinpol	1617.00		NIST Webbook

rinpol	1621.00		NIST Webbook
rinpol	1570.00		NIST Webbook
rinpol	1608.00		NIST Webbook
rinpol	1570.00		NIST Webbook
rinpol	1567.00		NIST Webbook
rinpol	1612.00		NIST Webbook
rinpol	1621.00		NIST Webbook
rinpol	1567.00		NIST Webbook
rinpol	1609.00		NIST Webbook
rinpol	1608.00		NIST Webbook
rinpol	1609.00		NIST Webbook
rinpol	1562.00		NIST Webbook
rinpol	1608.00		NIST Webbook
ripol	2148.00		NIST Webbook
ripol	2148.00		NIST Webbook
tb	545.23	K	Cheméo Relay (1.0)
tf	304.65	K	Aqueous Solubility Prediction 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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point