butacarb

Inchi: InChI=1S/C16H25NO2/c1-15(2,3)11-8-12(16(4,5)6)10-13(9-11)19-14(18)17-7/h8-10H,1-
InchiKey: SLZWBCGZQRRUNG-UHFFFAOYSA-N
Formula: C16H25NO2
SMILES: CNC(=O)Oc1cc(C(C)(C)C)cc(C(C)(C)C)c1
Mol. weight [g/mol]: 263.38

Physical Properties

Property code	Value	Unit	Source
gf	38.14	kJ/mol	Joback Method
hf	-368.81	kJ/mol	Joback Method
hfus	23.52	kJ/mol	Joback Method
hvap	67.81	kJ/mol	Joback Method
log10ws	-4.24		Estimated Solubility Method
log10ws	-4.24		Aqueous Solubility Prediction Method
logp	4.000		Crippen Method
mcvol	229.960	ml/mol	McGowan Method
pc	1801.56	kPa	Joback Method
tb	722.12	K	Joback Method
tc	939.01	K	Joback Method
tf	451.20	K	Joback Method
vc	0.861	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	661.84	J/mol×K	722.12	Joback Method
cpg	679.07	J/mol×K	758.27	Joback Method
cpg	695.12	J/mol×K	794.42	Joback Method
cpg	710.07	J/mol×K	830.57	Joback Method
cpg	723.98	J/mol×K	866.72	Joback Method
cpg	736.94	J/mol×K	902.86	Joback Method
cpg	749.00	J/mol×K	939.01	Joback Method

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
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume