Bromobutide

Other names: Butanamide, 2-bromo-3,3-dimethyl-N-(1-methyl-1-phenylethyl)-
Inchi: InChI=1S/C15H22BrNO/c1-14(2,3)12(16)13(18)17-15(4,5)11-9-7-6-8-10-11/h6-10,12H,1
InchiKey: WZDDLAZXUYIVMU-UHFFFAOYSA-N
Formula: C15H22BrNO
SMILES: CC(C)(NC(=O)C(Br)C(C)(C)C)c1ccccc1
Mol. weight [g/mol]: 312.25
CAS: 74712-19-9

Physical Properties

Property code	Value	Unit	Source
gf	165.86	kJ/mol	Joback Method
hf	-171.96	kJ/mol	Joback Method
hfus	22.28	kJ/mol	Joback Method
hvap	67.90	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	3.848		Crippen Method
mcvol	227.500	ml/mol	McGowan Method
pc	2191.78	kPa	Joback Method
rinpol	1879.00		NIST Webbook
rinpol	1887.00		NIST Webbook
rinpol	1912.20		NIST Webbook
rinpol	1887.00		NIST Webbook
rinpol	1879.00		NIST Webbook
rinpol	1912.20		NIST Webbook
tb	732.58	K	Joback Method
tc	968.71	K	Joback Method
tf	437.46	K	Joback Method
vc	0.843	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.72	J/mol×K	732.58	Joback Method
cpg	639.93	J/mol×K	771.94	Joback Method

cpg	654.87	J/mol×K	811.29	Joback Method
cpg	668.68	J/mol×K	850.65	Joback Method
cpg	681.49	J/mol×K	890.00	Joback Method
cpg	693.43	J/mol×K	929.36	Joback Method
cpg	704.64	J/mol×K	968.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74712199&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume