Bromobutide-debromo

Inchi: InChI=1S/C15H23NO/c1-14(2,3)11-13(17)16-15(4,5)12-9-7-6-8-10-12/h6-10H,11H2,1-5H
InchiKey: XYWRDHBULARJNY-UHFFFAOYSA-N
Formula: C15H23NO
SMILES: CC(C)(C)CC(=O)NC(C)(C)c1ccccc1
Mol. weight [g/mol]: 233.35

Physical Properties

Property code	Value	Unit	Source
gf	153.98	kJ/mol	Joback Method
hf	-193.01	kJ/mol	Joback Method
hfus	20.52	kJ/mol	Joback Method
hvap	61.85	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	3.474		Crippen Method
mcvol	210.000	ml/mol	McGowan Method
pc	2041.91	kPa	Joback Method
rinpol	1691.00		NIST Webbook
rinpol	1691.00		NIST Webbook
rinpol	1697.00		NIST Webbook
tb	666.86	K	Joback Method
tc	888.19	K	Joback Method
tf	392.66	K	Joback Method
vc	0.786	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.73	J/mol×K	666.86	Joback Method
cpg	598.64	J/mol×K	703.75	Joback Method
cpg	615.25	J/mol×K	740.64	Joback Method
cpg	630.64	J/mol×K	777.52	Joback Method
cpg	644.91	J/mol×K	814.41	Joback Method
cpg	658.18	J/mol×K	851.30	Joback Method
cpg	670.55	J/mol×K	888.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R197363&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