Propanamide, N,N-dihexyl-2-bromo-

Inchi: InChI=1S/C15H30BrNO/c1-4-6-8-10-12-17(15(18)14(3)16)13-11-9-7-5-2/h14H,4-13H2,1-
InchiKey: WRVBRLZMYIGDCH-UHFFFAOYSA-N
Formula: C15H30BrNO
SMILES: CCCCCCN(CCCCCC)C(=O)C(C)Br
Mol. weight [g/mol]: 320.31

Physical Properties

Property code	Value	Unit	Source
gf	69.16	kJ/mol	Joback Method
hf	-376.93	kJ/mol	Joback Method
hfus	40.99	kJ/mol	Joback Method
hvap	63.82	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	4.759		Crippen Method
mcvol	251.260	ml/mol	McGowan Method
pc	1574.70	kPa	Joback Method
rinpol	1943.00		NIST Webbook
rinpol	1943.00		NIST Webbook
tb	674.63	K	Joback Method
tc	854.99	K	Joback Method
tf	386.01	K	Joback Method
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.98	J/mol×K	674.63	Joback Method
cpg	701.15	J/mol×K	704.69	Joback Method
cpg	717.45	J/mol×K	734.75	Joback Method
cpg	732.93	J/mol×K	764.81	Joback Method
cpg	747.62	J/mol×K	794.87	Joback Method
cpg	761.56	J/mol×K	824.93	Joback Method
cpg	774.80	J/mol×K	854.99	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308373&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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