Propanamide, N,N-diheptyl-2-bromo-

Inchi: InChI=1S/C17H34BrNO/c1-4-6-8-10-12-14-19(17(20)16(3)18)15-13-11-9-7-5-2/h16H,4-1
InchiKey: RRKJZCUZIGJJIJ-UHFFFAOYSA-N
Formula: C17H34BrNO
SMILES: CCCCCCCN(CCCCCCC)C(=O)C(C)Br
Mol. weight [g/mol]: 348.36

Physical Properties

Property code	Value	Unit	Source
gf	86.00	kJ/mol	Joback Method
hf	-418.21	kJ/mol	Joback Method
hfus	46.17	kJ/mol	Joback Method
hvap	68.27	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	5.539		Crippen Method
mcvol	279.440	ml/mol	McGowan Method
pc	1359.63	kPa	Joback Method
rinpol	2141.00		NIST Webbook
tb	720.39	K	Joback Method
tc	900.24	K	Joback Method
tf	408.55	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	797.26	J/mol×K	720.39	Joback Method
cpg	815.14	J/mol×K	750.37	Joback Method
cpg	832.12	J/mol×K	780.34	Joback Method
cpg	848.24	J/mol×K	810.32	Joback Method
cpg	863.55	J/mol×K	840.29	Joback Method
cpg	878.08	J/mol×K	870.27	Joback Method
cpg	891.88	J/mol×K	900.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308376&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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