Propanamide, n-heptyl-n-octyl-2-bromo-

Inchi: InChI=1S/C18H36BrNO/c1-4-6-8-10-12-14-16-20(18(21)17(3)19)15-13-11-9-7-5-2/h17H,
InchiKey: AKYXBWMBRGAFJW-UHFFFAOYSA-N
Formula: C18H36BrNO
SMILES: CCCCCCCCN(CCCCCCC)C(=O)C(C)Br
Mol. weight [g/mol]: 362.39

Physical Properties

Property code	Value	Unit	Source
gf	94.42	kJ/mol	Joback Method
hf	-438.85	kJ/mol	Joback Method
hfus	48.76	kJ/mol	Joback Method
hvap	70.50	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	5.929		Crippen Method
mcvol	293.530	ml/mol	McGowan Method
pc	1268.25	kPa	Joback Method
rinpol	2241.00		NIST Webbook
rinpol	2241.00		NIST Webbook
tb	743.27	K	Joback Method
tc	923.63	K	Joback Method
tf	419.82	K	Joback Method
vc	1.123	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	855.52	J/mol×K	743.27	Joback Method
cpg	873.75	J/mol×K	773.33	Joback Method
cpg	891.06	J/mol×K	803.39	Joback Method
cpg	907.50	J/mol×K	833.45	Joback Method
cpg	923.10	J/mol×K	863.51	Joback Method
cpg	937.90	J/mol×K	893.57	Joback Method
cpg	951.97	J/mol×K	923.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308377&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