Pentanamide, N,N-diheptyl-5-bromo-

Inchi: InChI=1S/C19H38BrNO/c1-3-5-7-9-13-17-21(18-14-10-8-6-4-2)19(22)15-11-12-16-20/h3
InchiKey: IPGHIRQAGPYPHE-UHFFFAOYSA-N
Formula: C19H38BrNO
SMILES: CCCCCCCN(CCCCCCC)C(=O)CCCCBr
Mol. weight [g/mol]: 376.42

Physical Properties

Property code	Value	Unit	Source
gf	105.28	kJ/mol	Joback Method
hf	-454.21	kJ/mol	Joback Method
hfus	54.87	kJ/mol	Joback Method
hvap	73.11	kJ/mol	Joback Method
log10ws	-6.55		Crippen Method
logp	6.321		Crippen Method
mcvol	307.620	ml/mol	McGowan Method
pc	1179.28	kPa	Joback Method
rinpol	2463.00		NIST Webbook
tb	766.59	K	Joback Method
tc	946.64	K	Joback Method
tf	446.09	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	914.30	J/mol×K	766.59	Joback Method
cpg	932.74	J/mol×K	796.60	Joback Method
cpg	950.26	J/mol×K	826.61	Joback Method
cpg	966.89	J/mol×K	856.62	Joback Method
cpg	982.70	J/mol×K	886.62	Joback Method
cpg	997.71	J/mol×K	916.63	Joback Method
cpg	1011.99	J/mol×K	946.64	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308263&Units=SI

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