Hexanamide, N,N-diheptyl-6-bromo-

Inchi: InChI=1S/C20H40BrNO/c1-3-5-7-9-14-18-22(19-15-10-8-6-4-2)20(23)16-12-11-13-17-21
InchiKey: PWMMILRBWJLITN-UHFFFAOYSA-N
Formula: C20H40BrNO
SMILES: CCCCCCCN(CCCCCCC)C(=O)CCCCCBr
Mol. weight [g/mol]: 390.44

Physical Properties

Property code	Value	Unit	Source
gf	113.70	kJ/mol	Joback Method
hf	-474.85	kJ/mol	Joback Method
hfus	57.46	kJ/mol	Joback Method
hvap	75.34	kJ/mol	Joback Method
log10ws	-6.97		Crippen Method
logp	6.711		Crippen Method
mcvol	321.710	ml/mol	McGowan Method
pc	1105.21	kPa	Joback Method
rinpol	2501.00		NIST Webbook
tb	789.47	K	Joback Method
tc	971.53	K	Joback Method
tf	457.36	K	Joback Method
vc	1.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	974.49	J/mol×K	789.47	Joback Method
cpg	993.34	J/mol×K	819.81	Joback Method
cpg	1011.23	J/mol×K	850.16	Joback Method
cpg	1028.22	J/mol×K	880.50	Joback Method
cpg	1044.36	J/mol×K	910.84	Joback Method
cpg	1059.68	J/mol×K	941.18	Joback Method
cpg	1074.25	J/mol×K	971.53	Joback Method

Sources

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=U308651&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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