Hexanamide, N,N-bis(2-ethylhexyl)-6-bromo-

Inchi: InChI=1S/C22H44BrNO/c1-5-9-14-20(7-3)18-24(19-21(8-4)15-10-6-2)22(25)16-12-11-13
InchiKey: KDQYJOXEUADVMC-UHFFFAOYSA-N
Formula: C22H44BrNO
SMILES: CCCCC(CC)CN(CC(CC)CCCC)C(=O)CCCCCBr
Mol. weight [g/mol]: 418.50

Physical Properties

Property code	Value	Unit	Source
gf	125.66	kJ/mol	Joback Method
hf	-526.69	kJ/mol	Joback Method
hfus	55.59	kJ/mol	Joback Method
hvap	79.01	kJ/mol	Joback Method
log10ws	-7.33		Crippen Method
logp	7.203		Crippen Method
mcvol	349.890	ml/mol	McGowan Method
pc	986.40	kPa	Joback Method
rinpol	2469.00		NIST Webbook
rinpol	2469.00		NIST Webbook
tb	834.35	K	Joback Method
tc	1023.65	K	Joback Method
tf	449.90	K	Joback Method
vc	1.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1098.30	J/mol×K	834.35	Joback Method
cpg	1118.18	J/mol×K	865.90	Joback Method
cpg	1136.99	J/mol×K	897.45	Joback Method
cpg	1154.81	J/mol×K	929.00	Joback Method
cpg	1171.67	J/mol×K	960.55	Joback Method
cpg	1187.65	J/mol×K	992.10	Joback Method
cpg	1202.81	J/mol×K	1023.65	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=U308650&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