Pentanamide, N,N-bis(2-ethylhexyl)-5-bromo-

Inchi: InChI=1S/C21H42BrNO/c1-5-9-13-19(7-3)17-23(21(24)15-11-12-16-22)18-20(8-4)14-10-

InchiKey: LUNGCQXCRGMSAN-UHFFFAOYSA-N

Formula: C21H42BrNO

SMILES: CCCCC(CC)CN(CC(CC)CCCC)C(=O)CCCCBr

Mol. weight [g/mol]: 404.47

Physical Properties

Property code	Value	Unit	Source
gf	117.24	kJ/mol	Joback Method
hf	-506.05	kJ/mol	Joback Method
hfus	53.00	kJ/mol	Joback Method
hvap	76.79	kJ/mol	Joback Method
log10ws	-6.91		Crippen Method
logp	6.813		Crippen Method
mcvol	335.800	ml/mol	McGowan Method
pc	1048.69	kPa	Joback Method
rinpol	2431.00		NIST Webbook
tb	811.47	K	Joback Method
tc	997.94	K	Joback Method
tf	438.63	K	Joback Method
vc	1.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1036.46	J/mol×K	811.47	Joback Method
cpg	1055.94	J/mol×K	842.55	Joback Method
cpg	1074.38	J/mol×K	873.63	Joback Method
cpg	1091.85	J/mol×K	904.70	Joback Method
cpg	1108.41	J/mol×K	935.78	Joback Method
cpg	1124.10	J/mol×K	966.86	Joback Method
cpg	1138.97	J/mol×K	997.94	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=U308262&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