

Propanamide, N,N-bis(2-ethylhexyl)-2-bromo-

Inchi:	InChI=1S/C19H38BrNO/c1-6-10-12-17(8-3)14-21(19(22)16(5)20)15-18(9-4)13-11-7-2/h1
InchiKey:	UJEAGNRTIMDECU-UHFFFAOYSA-N
Formula:	C19H38BrNO
SMILES:	CCCCC(CC)CN(CC(CC)CCCC)C(=O)C(C)Br
Mol. weight [g/mol]:	376.42

Physical Properties

Property code	Value	Unit	Source
gf	97.96	kJ/mol	Joback Method
hf	-470.05	kJ/mol	Joback Method
hfus	44.30	kJ/mol	Joback Method
hvap	71.95	kJ/mol	Joback Method
log10ws	-6.18		Crippen Method
logp	6.031		Crippen Method
mvol	307.620	ml/mol	McGowan Method
pc	1198.96	kPa	Joback Method
rmpol	2114.00		NIST Webbook
rmpol	2114.00		NIST Webbook
tb	765.27	K	Joback Method
tc	949.87	K	Joback Method
tf	401.09	K	Joback Method
vc	1.167	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	915.72	J/molxK	765.27	Joback Method
cpg	934.66	J/molxK	796.04	Joback Method
cpg	952.60	J/molxK	826.80	Joback Method
cpg	969.59	J/molxK	857.57	Joback Method
cpg	985.68	J/molxK	888.34	Joback Method
cpg	1000.92	J/molxK	919.11	Joback Method
cpg	1015.36	J/molxK	949.87	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U308375&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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