

Bromoacetamide, N,N-bis(2-ethylhexyl)-

Inchi:	InChI=1S/C18H36BrNO/c1-5-9-11-16(7-3)14-20(18(21)13-19)15-17(8-4)12-10-6-2/h16-1
InchiKey:	RDTFKQQQEZVEJP-UHFFFAOYSA-N
Formula:	C18H36BrNO
SMILES:	CCCCC(CC)CN(CC(CC)CCCC)C(=O)CBr
Mol. weight [g/mol]:	362.39

Physical Properties

Property code	Value	Unit	Source
gf	91.98	kJ/mol	Joback Method
hf	-444.13	kJ/mol	Joback Method
hfus	45.23	kJ/mol	Joback Method
hvap	70.11	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	5.643		Crippen Method
mcvol	293.530	ml/mol	McGowan Method
pc	1275.51	kPa	Joback Method
rinpol	2127.00		NIST Webbook
rinpol	2127.00		NIST Webbook
tb	742.83	K	Joback Method
tc	924.99	K	Joback Method
tf	404.82	K	Joback Method
vc	1.117	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	855.99	J/mol×K	742.83	Joback Method
cpg	874.42	J/mol×K	773.19	Joback Method
cpg	891.90	J/mol×K	803.55	Joback Method
cpg	908.48	J/mol×K	833.91	Joback Method
cpg	924.20	J/mol×K	864.27	Joback Method
cpg	939.11	J/mol×K	894.63	Joback Method
cpg	953.24	J/mol×K	924.99	Joback Method

Sources

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=U308170&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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