

Bromacetamide, N-tetradecyl-

Inchi:	InChI=1S/C16H32BrNO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-18-16(19)15-17/h2-15H2,1H
InchiKey:	ZTUQVBZIIWWFOFJ-UHFFFAOYSA-N
Formula:	C16H32BrNO
SMILES:	CCCCCCCCCCCCCNC(=O)CBr
Mol. weight [g/mol]:	334.33

Physical Properties

Property code	Value	Unit	Source
gf	58.63	kJ/mol	Joback Method
hf	-406.35	kJ/mol	Joback Method
hfus	49.18	kJ/mol	Joback Method
hvap	70.83	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	5.199		Crippen Method
mvol	265.350	ml/mol	McGowan Method
pc	1469.10	kPa	Joback Method
rinpol	2346.00		NIST Webbook
rinpol	2346.00		NIST Webbook
tb	735.68	K	Joback Method
tc	917.68	K	Joback Method
tf	432.47	K	Joback Method
vc	1.034	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	759.77	J/molxK	735.68	Joback Method
cpg	776.46	J/molxK	766.01	Joback Method
cpg	792.31	J/molxK	796.35	Joback Method
cpg	807.35	J/molxK	826.68	Joback Method
cpg	821.64	J/molxK	857.01	Joback Method
cpg	835.19	J/molxK	887.34	Joback Method
cpg	848.06	J/molxK	917.68	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=U407082&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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