Bromoacetamide, N,N-diundecyl-

Inchi: InChI=1S/C24H48BrNO/c1-3-5-7-9-11-13-15-17-19-21-26(24(27)23-25)22-20-18-16-14-1
InchiKey: GMTOKSHJAROLMG-UHFFFAOYSA-N
Formula: C24H48BrNO
SMILES: CCCCCCCCCCCN(CCCCCCCCCCC)C(=O)CBr
Mol. weight [g/mol]: 446.55

Physical Properties

Property code	Value	Unit	Source
gf	147.38	kJ/mol	Joback Method
hf	-557.41	kJ/mol	Joback Method
hfus	67.82	kJ/mol	Joback Method
hvap	84.24	kJ/mol	Joback Method
log10ws	-8.65		Crippen Method
logp	8.271		Crippen Method
mcvol	378.070	ml/mol	McGowan Method
pc	869.14	kPa	Joback Method
rinpol	3016.00		NIST Webbook
tb	880.99	K	Joback Method
tc	1078.73	K	Joback Method
tf	502.44	K	Joback Method
vc	1.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1223.29	J/mol×K	880.99	Joback Method
cpg	1244.20	J/mol×K	913.95	Joback Method
cpg	1263.98	J/mol×K	946.90	Joback Method
cpg	1282.69	J/mol×K	979.86	Joback Method
cpg	1300.41	J/mol×K	1012.82	Joback Method
cpg	1317.21	J/mol×K	1045.78	Joback Method
cpg	1333.16	J/mol×K	1078.73	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=U308176&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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