

n-bromoacetamide

Inchi:	InChI=1S/C2H4BrNO/c1-2(5)4-3/h1H3,(H,4,5)
InchiKey:	VBTQNRFWXBZXQR-UHFFFAOYSA-N
Formula:	C2H4BrNO
SMILES:	CC(=O)NBr
Mol. weight [g/mol]:	137.96
CAS:	79-15-2

Physical Properties

Property code	Value	Unit	Source
af	0.4517		Cheméo Relay (1.0)
gf	-59.25	kJ/mol	Joback Method
hf	-113.58	kJ/mol	Cheméo Relay (1.0)
hfus	12.92	kJ/mol	Joback Method
hvap	54.22	kJ/mol	Cheméo Relay (1.0)
ie	9.77	eV	Cheméo Relay (1.0)
log10ws	-0.02		Cheméo Relay (1.0)
logp	0.432		Crippen Method
mcvol	68.090	ml/mol	McGowan Method
pc	6249.12	kPa	Joback Method
tb	443.62	K	Cheméo Relay (1.0)
tc	707.97	K	Cheméo Relay (1.0)
tf	376.90	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)
vc	0.254	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	1.54100e+01
Coeff. B	2.80220e-01

Coeff. C	-1.86300e-04
Coeff. D	4.81600e-08
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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