

Hexanehydroxamic acid

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C6H13NO2/c1-2-3-4-5-6(8)7-9/h9H,2-5H2,1H3,(H,7,8)

FWPKDESKJMMUSR-UHFFFAOYSA-N

C6H13NO2

CCCCC(=O)NO

131.17

Physical Properties

Property code	Value	Unit	Source
af	0.7044		Cheméo Relay (1.0)
gf	-176.71	kJ/mol	Joback Method
hf	-393.09	kJ/mol	Cheméo Relay (1.0)
hfus	22.08	kJ/mol	Joback Method
hvap	78.46	kJ/mol	Cheméo Relay (1.0)
ie	10.03	eV	Cheméo Relay (1.0)
log10ws	-0.46		Cheméo Relay (1.0)
logp	1.072		Crippen Method
mcvol	112.820	ml/mol	McGowan Method
pc	3782.33	kPa	Joback Method
tb	473.05	K	Cheméo Relay (1.0)
tc	710.09	K	Cheméo Relay (1.0)
tf	342.33	K	Cheméo Relay (1.0)
vc	0.425	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.22	J/mol×K	532.90	Joback Method
cpg	275.60	J/mol×K	561.92	Joback Method
cpg	284.56	J/mol×K	590.95	Joback Method
cpg	293.13	J/mol×K	619.97	Joback Method
cpg	301.31	J/mol×K	648.99	Joback Method
cpg	309.11	J/mol×K	678.02	Joback Method
cpg	316.55	J/mol×K	707.04	Joback Method

Sources

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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C4312930

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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