

D-Glucose, dihexylthioacetal

Other names:	D-Glucose, dihexyl mercaptal (D)-glucose dihexyl dithioacetal
Inchi:	InChI=1S/C18H38O5S2/c1-3-5-7-9-11-24-18(25-12-10-8-6-4-2)17(23)16(22)15(21)14(20)
InchiKey:	NVZRRIMRHXQLPB-UHFFFAOYSA-N
Formula:	C18H38O5S2
SMILES:	CCCCCSC(SCCCCCC)C(O)C(O)C(O)C(O)CO
Mol. weight [g/mol]:	398.62
CAS:	115395-54-5

Physical Properties

Property code	Value	Unit	Source
gf	-529.38	kJ/mol	Joback Method
hf	-1118.66	kJ/mol	Joback Method
hfus	53.46	kJ/mol	Joback Method
hvap	150.75	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	2.375		Crippen Method
mvol	326.530	ml/mol	McGowan Method
pc	1718.88	kPa	Joback Method
tb	1207.50	K	Joback Method
tc	1580.60	K	Joback Method
tf	590.52	K	Joback Method
vc	1.216	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1161.91	J/molxK	1207.50	Joback Method
cpg	1175.15	J/molxK	1269.68	Joback Method
cpg	1186.04	J/molxK	1331.87	Joback Method
cpg	1194.87	J/molxK	1394.05	Joback Method
cpg	1201.92	J/molxK	1456.23	Joback Method
cpg	1207.47	J/molxK	1518.41	Joback Method
cpg	1211.79	J/molxK	1580.60	Joback Method

Sources

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=C115395545&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hfust:	Enthalpy of fusion at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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