D-GLUCOSE, DIHEXYL MERCAPTAL

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: CCCCCCSC(SCCCCCC)C(O)C(O)C(O)C(O)CO
Mol. weight [g/mol]: 398.63

Physical Properties

Property code	Value	Unit	Source
hfus	53.46	kJ/mol	Joback Method
logp	2.375		Crippen Method
mcvol	326.530	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1161.91	J/mol×K	1207.50	Joback Method
cpg	1175.15	J/mol×K	1269.68	Joback Method
cpg	1186.04	J/mol×K	1331.87	Joback Method
cpg	1194.87	J/mol×K	1394.05	Joback Method
cpg	1201.92	J/mol×K	1456.23	Joback Method
cpg	1207.47	J/mol×K	1518.41	Joback Method
cpg	1211.79	J/mol×K	1580.60	Joback Method
hfust	44.60	kJ/mol	377.00	NIST Webbook

Sources

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?ID=C115395545&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume