L-fucose, acetylated diethyldithioacetal derivative

Inchi: InChI=1S/C18H30O8S2/c1-8-27-18(28-9-2)17(26-14(7)22)16(25-13(6)21)15(24-12(5)20)

InchiKey: IGZAPMUTZWRKTE-OOOSANSDSA-N

Formula: C18H30O8S2

SMILES: CCSC(SCC)C(OC(C)=O)C(OC(C)=O)C(OC(C)=O)C(C)OC(C)=O

Mol. weight [g/mol]: 438.56

Physical Properties

Property code	Value	Unit	Source
gf	-780.96	kJ/mol	Joback Method
hf	-1336.71	kJ/mol	Joback Method
hfus	44.17	kJ/mol	Joback Method
hvap	103.98	kJ/mol	Joback Method
log10ws	-3.63		Crippen Method
logp	2.565		Crippen Method
mcvol	326.940	ml/mol	McGowan Method
pc	1384.02	kPa	Joback Method
rinpol	2252.00		NIST Webbook
rinpol	2252.00		NIST Webbook
tb	1051.76	K	Joback Method
tc	1288.34	K	Joback Method
tf	575.06	K	Joback Method
vc	1.218	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1047.17	J/mol×K	1051.76	Joback Method
cpg	1054.69	J/mol×K	1091.19	Joback Method
cpg	1059.93	J/mol×K	1130.62	Joback Method
cpg	1062.86	J/mol×K	1170.05	Joback Method
cpg	1063.42	J/mol×K	1209.48	Joback Method
cpg	1061.59	J/mol×K	1248.91	Joback Method
cpg	1057.31	J/mol×K	1288.34	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R502859&Units=SI

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

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