D-mannose, acetylated diethyldithioacetal derivative

Inchi: InChI=1S/C20H32O10S2/c1-8-31-20(32-9-2)19(30-15(7)25)18(29-14(6)24)17(28-13(5)23

InchiKey: NFCGRENOZDIGBW-YRXWBPOGSA-N

Formula: C20H32O10S2

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

Mol. weight [g/mol]: 496.59

Physical Properties

Property code	Value	Unit	Source
gf	-998.04	kJ/mol	Joback Method
hf	-1622.79	kJ/mol	Joback Method
hfus	52.14	kJ/mol	Joback Method
hvap	117.59	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	2.109		Crippen Method
mcvol	362.560	ml/mol	McGowan Method
pc	1245.09	kPa	Joback Method
rinpol	2469.00		NIST Webbook
rinpol	2469.00		NIST Webbook
tb	1173.81	K	Joback Method
tc	1441.98	K	Joback Method
tf	669.76	K	Joback Method
vc	1.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1174.07	J/mol×K	1173.81	Joback Method
cpg	1173.24	J/mol×K	1218.50	Joback Method
cpg	1168.81	J/mol×K	1263.20	Joback Method
cpg	1160.71	J/mol×K	1307.89	Joback Method
cpg	1148.85	J/mol×K	1352.59	Joback Method
cpg	1133.16	J/mol×K	1397.28	Joback Method
cpg	1113.55	J/mol×K	1441.98	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=R502795&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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