L-Mannose, 6-deoxy-, dioctyl mercaptal

Other names: (l)-rhamnose dioctyl dithioacetal
Inchi: InChI=1S/C22H46O4S2/c1-4-6-8-10-12-14-16-27-22(21(26)20(25)19(24)18(3)23)28-17-1
InchiKey: SDOOHQUJOHBBFO-UHFFFAOYSA-N
Formula: C22H46O4S2
SMILES: CCCCCCCCSC(SCCCCCCCC)C(O)C(O)C(O)C(C)O
Mol. weight [g/mol]: 438.73
CAS: 115395-63-6

Physical Properties

Property code	Value	Unit	Source
gf	-358.88	kJ/mol	Joback Method
hf	-1048.99	kJ/mol	Joback Method
hfus	59.73	kJ/mol	Joback Method
hvap	142.98	kJ/mol	Joback Method
log10ws	-6.91		Crippen Method
logp	4.963		Crippen Method
mcvol	377.020	ml/mol	McGowan Method
pc	1198.96	kPa	Joback Method
tb	1206.84	K	Joback Method
tc	1576.62	K	Joback Method
tf	574.78	K	Joback Method
vc	1.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1364.22	J/mol×K	1206.84	Joback Method
cpg	1380.84	J/mol×K	1268.47	Joback Method
cpg	1394.84	J/mol×K	1330.10	Joback Method
cpg	1406.52	J/mol×K	1391.73	Joback Method
cpg	1416.22	J/mol×K	1453.36	Joback Method
cpg	1424.26	J/mol×K	1514.99	Joback Method
cpg	1430.97	J/mol×K	1576.62	Joback Method
hfust	54.70	kJ/mol	387.90	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C115395636&Units=SI
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

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