l-Arabinose, dihexyl mercaptal

Other names: (L)-arabinose dihexyl dithioacetal
Inchi: InChI=1S/C17H36O4S2/c1-3-5-7-9-11-22-17(23-12-10-8-6-4-2)16(21)15(20)14(19)13-18
InchiKey: UUJAXMJAXUORFA-UHFFFAOYSA-N
Formula: C17H36O4S2
SMILES: CCCCCCSC(SCCCCCC)C(O)C(O)C(O)CO
Mol. weight [g/mol]: 368.60
CAS: 123390-03-4

Physical Properties

Property code	Value	Unit	Source
gf	-398.54	kJ/mol	Joback Method
hf	-940.51	kJ/mol	Joback Method
hfus	50.31	kJ/mol	Joback Method
hvap	132.23	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	3.014		Crippen Method
mcvol	306.570	ml/mol	McGowan Method
pc	1713.19	kPa	Joback Method
tb	1092.88	K	Joback Method
tc	1370.60	K	Joback Method
tf	533.43	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1057.74	J/mol×K	1092.88	Joback Method
cpg	1070.82	J/mol×K	1139.17	Joback Method
cpg	1082.34	J/mol×K	1185.45	Joback Method
cpg	1092.40	J/mol×K	1231.74	Joback Method
cpg	1101.11	J/mol×K	1278.03	Joback Method
cpg	1108.58	J/mol×K	1324.31	Joback Method
cpg	1114.90	J/mol×K	1370.60	Joback Method
hfust	39.20	kJ/mol	367.20	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C123390034&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