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

Physical Properties

Property code	Value	Unit	Source
hfus	50.31	kJ/mol	Joback Method
log10ws	-3.68		Cheméo Relay (1.0)
logp	3.014		Crippen Method
mcvol	306.570	ml/mol	McGowan Method
tf	367.98	K	Cheméo Relay (1.0)

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

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=C123390034&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point