

L-arabinose, acetylated diethyldithioacetal derivative

Inchi:	InChI=1S/C17H28O8S2/c1-7-26-17(27-8-2)16(25-13(6)21)15(24-12(5)20)14(23-11(4)19)
InchiKey:	OGSWVSGRSHUBOP-HRCADAONSA-N
Formula:	C17H28O8S2
SMILES:	CCSC(SCC)C(OC(C)=O)C(OC(C)=O)C(COC(C)=O)OC(C)=O
Mol. weight [g/mol]:	424.53

Physical Properties

Property code	Value	Unit	Source
gf	-786.94	kJ/mol	Joback Method
hf	-1310.79	kJ/mol	Joback Method
hfus	45.10	kJ/mol	Joback Method
hvap	102.14	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	2.177		Crippen Method
mcvol	312.850	ml/mol	McGowan Method
pc	1479.29	kPa	Joback Method
rinsol	2252.00		NIST Webbook
tb	1029.32	K	Joback Method
tc	1261.82	K	Joback Method
tf	578.79	K	Joback Method
vc	1.167	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	989.20	J/molxK	1029.32	Joback Method
cpg	997.18	J/molxK	1068.07	Joback Method
cpg	1003.04	J/molxK	1106.82	Joback Method
cpg	1006.75	J/molxK	1145.57	Joback Method
cpg	1008.26	J/molxK	1184.32	Joback Method
cpg	1007.53	J/molxK	1223.07	Joback Method
cpg	1004.52	J/molxK	1261.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R502839&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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