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
rinpol	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	m3/kmol	Joback Method

Temperature Dependent Properties

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

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R502839&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

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

Latest version available from:
https://www.chemeo.com/cid/61-006-7/L-arabinose-acetylated-diethyldithioacetal-derivative.pdf
Generated by Cheméo on 2024-10-12 08:18:25.035349713 +0000 UTC m=+3301967.672318961.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.