Diethylmalonic acid, di(tetrahydrofurfuryl) ester

Inchi: InChI=1S/C17H28O6/c1-3-17(4-2,15(18)22-11-13-7-5-9-20-13)16(19)23-12-14-8-6-10-21

InchiKey: OCPSTBMCYRAGTA-UHFFFAOYSA-N

Formula: C17H28O6

SMILES: CCC(CC)(C(=O)OCC1CCCO1)C(=O)OCC1CCCO1

Mol. weight [g/mol]: 328.40

Physical Properties

Property code	Value	Unit	Source
gf	-471.88	kJ/mol	Joback Method
hf	-1035.60	kJ/mol	Joback Method
hfus	41.77	kJ/mol	Joback Method
hvap	79.99	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.237		Crippen Method
mcvol	255.290	ml/mol	McGowan Method
pc	1740.46	kPa	Joback Method
rinpol	2167.00		NIST Webbook
rinpol	2167.00		NIST Webbook
tb	822.17	K	Joback Method
tc	1038.47	K	Joback Method
tf	503.03	K	Joback Method
vc	0.949	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	844.57	J/mol×K	822.17	Joback Method
cpg	919.31	J/mol×K	1002.42	Joback Method
cpg	906.91	J/mol×K	966.37	Joback Method
cpg	893.30	J/mol×K	930.32	Joback Method
cpg	878.41	J/mol×K	894.27	Joback Method
cpg	862.18	J/mol×K	858.22	Joback Method
cpg	930.54	J/mol×K	1038.47	Joback Method
dvisc	0.0001062	Pa×s	822.17	Joback Method

dvisc	0.0001385	Pa×s	768.98	Joback Method
dvisc	0.0001881	Pa×s	715.79	Joback Method
dvisc	0.0002682	Pa×s	662.60	Joback Method
dvisc	0.0004068	Pa×s	609.41	Joback Method
dvisc	0.0006683	Pa×s	556.22	Joback Method
dvisc	0.0012196	Pa×s	503.03	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370649&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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