Diethylmalonic acid, tetrahydrofurfuryl undecyl ester

Inchi: InChI=1S/C23H42O5/c1-4-7-8-9-10-11-12-13-14-17-27-21(24)23(5-2,6-3)22(25)28-19-20

InchiKey: ZNOSFMMHZQJZJM-UHFFFAOYSA-N

Formula: C23H42O5

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

Mol. weight [g/mol]: 398.58

Physical Properties

Property code	Value	Unit	Source
gf	-371.79	kJ/mol	Joback Method
hf	-1087.92	kJ/mol	Joback Method
hfus	55.40	kJ/mol	Joback Method
hvap	88.57	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	5.589		Crippen Method
mcvol	344.820	ml/mol	McGowan Method
pc	1011.66	kPa	Joback Method
rinpol	2569.00		NIST Webbook
rinpol	2569.00		NIST Webbook
tb	917.22	K	Joback Method
tc	1123.88	K	Joback Method
tf	533.18	K	Joback Method
vc	1.323	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1182.75	J/mol×K	917.22	Joback Method
cpg	1201.38	J/mol×K	951.66	Joback Method
cpg	1218.65	J/mol×K	986.11	Joback Method
cpg	1234.61	J/mol×K	1020.55	Joback Method
cpg	1249.32	J/mol×K	1054.99	Joback Method
cpg	1262.85	J/mol×K	1089.44	Joback Method
cpg	1275.24	J/mol×K	1123.88	Joback Method
dvisc	0.0005620	Pa×s	533.18	Joback Method

dvisc	0.0002730	Pa×s	597.19	Joback Method
dvisc	0.0001526	Pa×s	661.19	Joback Method
dvisc	0.0000945	Pa×s	725.20	Joback Method
dvisc	0.0000632	Pa×s	789.21	Joback Method
dvisc	0.0000449	Pa×s	853.21	Joback Method
dvisc	0.0000335	Pa×s	917.22	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=U370646&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