Diethylmalonic acid, decyl tetrahydrofurfuryl ester

Inchi: InChI=1S/C22H40O5/c1-4-7-8-9-10-11-12-13-16-26-20(23)22(5-2,6-3)21(24)27-18-19-15

InchiKey: BNPDQFIZHQJOHO-UHFFFAOYSA-N

Formula: C22H40O5

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

Mol. weight [g/mol]: 384.55

Physical Properties

Property code	Value	Unit	Source
gf	-380.21	kJ/mol	Joback Method
hf	-1067.28	kJ/mol	Joback Method
hfus	52.81	kJ/mol	Joback Method
hvap	86.35	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	5.199		Crippen Method
mcvol	330.730	ml/mol	McGowan Method
pc	1076.39	kPa	Joback Method
rinpol	2471.00		NIST Webbook
rinpol	2471.00		NIST Webbook
tb	894.34	K	Joback Method
tc	1097.66	K	Joback Method
tf	521.91	K	Joback Method
vc	1.266	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1120.54	J/mol×K	894.34	Joback Method
cpg	1138.94	J/mol×K	928.23	Joback Method
cpg	1156.03	J/mol×K	962.11	Joback Method
cpg	1171.86	J/mol×K	996.00	Joback Method
cpg	1186.49	J/mol×K	1029.88	Joback Method
cpg	1199.97	J/mol×K	1063.77	Joback Method
cpg	1212.34	J/mol×K	1097.66	Joback Method
dvisc	0.0006388	Pa×s	521.91	Joback Method

dvisc	0.0003134	Pa×s	583.98	Joback Method
dvisc	0.0001763	Pa×s	646.05	Joback Method
dvisc	0.0001097	Pa×s	708.12	Joback Method
dvisc	0.0000737	Pa×s	770.20	Joback Method
dvisc	0.0000525	Pa×s	832.27	Joback Method
dvisc	0.0000392	Pa×s	894.34	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=U370645&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