Diethylmalonic acid, nonyl tetrahydrofurfuryl ester

Inchi: InChI=1S/C21H38O5/c1-4-7-8-9-10-11-12-15-25-19(22)21(5-2,6-3)20(23)26-17-18-14-13

InchiKey: ZCTZYXHWRMHOSZ-UHFFFAOYSA-N

Formula: C21H38O5

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

Mol. weight [g/mol]: 370.52

Physical Properties

Property code	Value	Unit	Source
gf	-388.63	kJ/mol	Joback Method
hf	-1046.64	kJ/mol	Joback Method
hfus	50.22	kJ/mol	Joback Method
hvap	84.12	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	4.809		Crippen Method
mcvol	316.640	ml/mol	McGowan Method
pc	1147.54	kPa	Joback Method
rinpol	2367.00		NIST Webbook
rinpol	2367.00		NIST Webbook
tb	871.46	K	Joback Method
tc	1072.29	K	Joback Method
tf	510.64	K	Joback Method
vc	1.210	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.90	J/mol×K	871.46	Joback Method
cpg	1077.10	J/mol×K	904.93	Joback Method
cpg	1094.04	J/mol×K	938.40	Joback Method
cpg	1109.76	J/mol×K	971.87	Joback Method
cpg	1124.31	J/mol×K	1005.35	Joback Method
cpg	1137.74	J/mol×K	1038.82	Joback Method
cpg	1150.10	J/mol×K	1072.29	Joback Method
dvisc	0.0007241	Pa×s	510.64	Joback Method

dvisc	0.0003589	Pa×s	570.78	Joback Method
dvisc	0.0002033	Pa×s	630.91	Joback Method
dvisc	0.0001271	Pa×s	691.05	Joback Method
dvisc	0.0000857	Pa×s	751.19	Joback Method
dvisc	0.0000613	Pa×s	811.32	Joback Method
dvisc	0.0000459	Pa×s	871.46	Joback Method

Sources

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=U370644&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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