Diethylmalonic acid, tetrahydrofurfuryl tridecyl ester

Inchi: InChI=1S/C25H46O5/c1-4-7-8-9-10-11-12-13-14-15-16-19-29-23(26)25(5-2,6-3)24(27)30

InchiKey: YDARTEYDJOOPQP-UHFFFAOYSA-N

Formula: C25H46O5

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

Mol. weight [g/mol]: 426.63

Physical Properties

Property code	Value	Unit	Source
gf	-354.95	kJ/mol	Joback Method
hf	-1129.20	kJ/mol	Joback Method
hfus	60.58	kJ/mol	Joback Method
hvap	93.03	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	6.369		Crippen Method
mcvol	373.000	ml/mol	McGowan Method
pc	898.56	kPa	Joback Method
rinpol	2759.00		NIST Webbook
rinpol	2759.00		NIST Webbook
tb	962.98	K	Joback Method
tc	1179.15	K	Joback Method
tf	555.72	K	Joback Method
vc	1.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1308.71	J/mol×K	962.98	Joback Method
cpg	1327.92	J/mol×K	999.01	Joback Method
cpg	1345.62	J/mol×K	1035.04	Joback Method
cpg	1361.89	J/mol×K	1071.07	Joback Method
cpg	1376.81	J/mol×K	1107.09	Joback Method
cpg	1390.44	J/mol×K	1143.12	Joback Method
cpg	1402.87	J/mol×K	1179.15	Joback Method
dvisc	0.0004315	Pa×s	555.72	Joback Method

dvisc	0.0002058	Pa×s	623.60	Joback Method
dvisc	0.0001135	Pa×s	691.47	Joback Method
dvisc	0.0000696	Pa×s	759.35	Joback Method
dvisc	0.0000463	Pa×s	827.23	Joback Method
dvisc	0.0000327	Pa×s	895.10	Joback Method
dvisc	0.0000243	Pa×s	962.98	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=U370648&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