Diethylmalonic acid, 3-methylpent-2-yl undecyl ester

Inchi: InChI=1S/C24H46O4/c1-7-11-12-13-14-15-16-17-18-19-27-22(25)24(9-3,10-4)23(26)28-
InchiKey: SDRMWGWDALUXKP-UHFFFAOYSA-N
Formula: C24H46O4
SMILES: CCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OC(C)C(C)CC
Mol. weight [g/mol]: 398.62

Physical Properties

Property code	Value	Unit	Source
gf	-318.68	kJ/mol	Joback Method
hf	-1047.60	kJ/mol	Joback Method
hfus	49.03	kJ/mol	Joback Method
hvap	85.26	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	6.845		Crippen Method
mcvol	363.900	ml/mol	McGowan Method
pc	867.60	kPa	Joback Method
rinpol	2367.00		NIST Webbook
rinpol	2367.00		NIST Webbook
tb	896.99	K	Joback Method
tc	1098.18	K	Joback Method
tf	476.98	K	Joback Method
vc	1.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1218.49	J/mol×K	896.99	Joback Method
cpg	1238.28	J/mol×K	930.52	Joback Method
cpg	1256.73	J/mol×K	964.05	Joback Method
cpg	1273.90	J/mol×K	997.59	Joback Method
cpg	1289.84	J/mol×K	1031.12	Joback Method
cpg	1304.59	J/mol×K	1064.65	Joback Method
cpg	1318.20	J/mol×K	1098.18	Joback Method
dvisc	0.0006687	Pa×s	476.98	Joback Method

dvisc	0.0002530	Pa×s	546.98	Joback Method
dvisc	0.0001193	Pa×s	616.98	Joback Method
dvisc	0.0000656	Pa×s	686.99	Joback Method
dvisc	0.0000403	Pa×s	756.99	Joback Method
dvisc	0.0000269	Pa×s	826.99	Joback Method
dvisc	0.0000191	Pa×s	896.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369736&Units=SI
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

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