Dimethylmalonic acid, 2-methylpent-3-yl tetradecyl ester

Inchi: InChI=1S/C25H48O4/c1-7-9-10-11-12-13-14-15-16-17-18-19-20-28-23(26)25(5,6)24(27)
InchiKey: JUFIXXXJDJNBPA-UHFFFAOYSA-N
Formula: C25H48O4
SMILES: CCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OC(CC)C(C)C
Mol. weight [g/mol]: 412.65

Physical Properties

Property code	Value	Unit	Source
gf	-310.26	kJ/mol	Joback Method
hf	-1068.24	kJ/mol	Joback Method
hfus	51.62	kJ/mol	Joback Method
hvap	87.48	kJ/mol	Joback Method
log10ws	-7.64		Crippen Method
logp	7.235		Crippen Method
mcvol	377.990	ml/mol	McGowan Method
pc	820.54	kPa	Joback Method
rinpol	2567.00		NIST Webbook
rinpol	2567.00		NIST Webbook
tb	919.87	K	Joback Method
tc	1126.52	K	Joback Method
tf	488.25	K	Joback Method
vc	1.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1281.85	J/mol×K	919.87	Joback Method
cpg	1302.06	J/mol×K	954.31	Joback Method
cpg	1320.85	J/mol×K	988.75	Joback Method
cpg	1338.27	J/mol×K	1023.20	Joback Method
cpg	1354.40	J/mol×K	1057.64	Joback Method
cpg	1369.27	J/mol×K	1092.08	Joback Method
cpg	1382.95	J/mol×K	1126.52	Joback Method
dvisc	0.0005773	Pa×s	488.25	Joback Method

dvisc	0.0002172	Pa×s	560.19	Joback Method
dvisc	0.0001021	Pa×s	632.12	Joback Method
dvisc	0.0000560	Pa×s	704.06	Joback Method
dvisc	0.0000343	Pa×s	776.00	Joback Method
dvisc	0.0000228	Pa×s	847.93	Joback Method
dvisc	0.0000162	Pa×s	919.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361799&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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