Dimethylmalonic acid, neopentyl tetradecyl ester

Inchi: InChI=1S/C24H46O4/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-27-21(25)24(5,6)22(26)2
InchiKey: RYCTXLGLFWKVDE-UHFFFAOYSA-N
Formula: C24H46O4
SMILES: CCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCC(C)(C)C
Mol. weight [g/mol]: 398.62

Physical Properties

Property code	Value	Unit	Source
gf	-310.96	kJ/mol	Joback Method
hf	-1045.79	kJ/mol	Joback Method
hfus	48.66	kJ/mol	Joback Method
hvap	84.74	kJ/mol	Joback Method
log10ws	-7.11		Crippen Method
logp	6.846		Crippen Method
mcvol	363.900	ml/mol	McGowan Method
pc	869.14	kPa	Joback Method
rinpol	2436.00		NIST Webbook
rinpol	2436.00		NIST Webbook
tb	894.64	K	Joback Method
tc	1095.43	K	Joback Method
tf	509.40	K	Joback Method
vc	1.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1217.75	J/mol×K	894.64	Joback Method
cpg	1304.18	J/mol×K	1061.97	Joback Method
cpg	1289.13	J/mol×K	1028.50	Joback Method
cpg	1273.03	J/mol×K	995.04	Joback Method
cpg	1255.80	J/mol×K	961.57	Joback Method
cpg	1237.40	J/mol×K	928.11	Joback Method
cpg	1318.25	J/mol×K	1095.43	Joback Method
dvisc	0.0000178	Pa×s	894.64	Joback Method

dvisc	0.0000247	Pa×s	830.43	Joback Method
dvisc	0.0000361	Pa×s	766.23	Joback Method
dvisc	0.0000568	Pa×s	702.02	Joback Method
dvisc	0.0000978	Pa×s	637.81	Joback Method
dvisc	0.0001900	Pa×s	573.61	Joback Method
dvisc	0.0004368	Pa×s	509.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361754&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