Dimethylmalonic acid, neopentyl pentadecyl ester

Inchi: InChI=1S/C25H48O4/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-28-22(26)25(5,6)23(2
InchiKey: MWFVGLDUTCWAOW-UHFFFAOYSA-N
Formula: C25H48O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCC(C)(C)C
Mol. weight [g/mol]: 412.65

Physical Properties

Property code	Value	Unit	Source
gf	-302.54	kJ/mol	Joback Method
hf	-1066.43	kJ/mol	Joback Method
hfus	51.25	kJ/mol	Joback Method
hvap	86.96	kJ/mol	Joback Method
log10ws	-7.53		Crippen Method
logp	7.236		Crippen Method
mcvol	377.990	ml/mol	McGowan Method
pc	821.95	kPa	Joback Method
rinpol	2535.00		NIST Webbook
tb	917.52	K	Joback Method
tc	1123.40	K	Joback Method
tf	520.67	K	Joback Method
vc	1.462	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1280.97	J/mol×K	917.52	Joback Method
cpg	1301.07	J/mol×K	951.83	Joback Method
cpg	1319.85	J/mol×K	986.15	Joback Method
cpg	1337.39	J/mol×K	1020.46	Joback Method
cpg	1353.77	J/mol×K	1054.78	Joback Method
cpg	1369.06	J/mol×K	1089.09	Joback Method
cpg	1383.33	J/mol×K	1123.40	Joback Method
dvisc	0.0003781	Pa×s	520.67	Joback Method
dvisc	0.0001631	Pa×s	586.81	Joback Method

dvisc	0.0000835	Pa×s	652.95	Joback Method
dvisc	0.0000483	Pa×s	719.10	Joback Method
dvisc	0.0000307	Pa×s	785.24	Joback Method
dvisc	0.0000209	Pa×s	851.38	Joback Method
dvisc	0.0000150	Pa×s	917.52	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361755&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