Diethylmalonic acid, heptyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C22H42O4/c1-8-11-12-13-14-15-25-19(23)22(9-2,10-3)20(24)26-17-18(4)16-2

InchiKey: VEHOWGRAGRKDMO-UHFFFAOYSA-N

Formula: C22H42O4

SMILES: CCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(C)CC(C)(C)C

Mol. weight [g/mol]: 370.57

Physical Properties

Property code	Value	Unit	Source
gf	-330.24	kJ/mol	Joback Method
hf	-1009.79	kJ/mol	Joback Method
hfus	39.96	kJ/mol	Joback Method
hvap	79.90	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	5.922		Crippen Method
mcvol	335.720	ml/mol	McGowan Method
pc	981.46	kPa	Joback Method
rinpol	2114.00		NIST Webbook
rinpol	2114.00		NIST Webbook
tb	848.44	K	Joback Method
tc	1042.65	K	Joback Method
tf	471.86	K	Joback Method
vc	1.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1093.57	J/mol×K	848.44	Joback Method
cpg	1177.39	J/mol×K	1010.28	Joback Method
cpg	1162.74	J/mol×K	977.91	Joback Method
cpg	1147.09	J/mol×K	945.54	Joback Method
cpg	1130.38	J/mol×K	913.18	Joback Method
cpg	1112.56	J/mol×K	880.81	Joback Method
cpg	1191.08	J/mol×K	1042.65	Joback Method
dvisc	0.0000227	Pa×s	848.44	Joback Method

dvisc	0.0000320	Pa×s	785.68	Joback Method
dvisc	0.0000478	Pa×s	722.91	Joback Method
dvisc	0.0000771	Pa×s	660.15	Joback Method
dvisc	0.0001375	Pa×s	597.39	Joback Method
dvisc	0.0002810	Pa×s	534.62	Joback Method
dvisc	0.0006945	Pa×s	471.86	Joback Method

Sources

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=U369479&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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