Diethylmalonic acid, 2-methylhex-3-yl 2-octyl ester

Inchi: InChI=1S/C22H42O4/c1-8-12-13-14-16-18(7)25-20(23)22(10-3,11-4)21(24)26-19(15-9-2
InchiKey: SKLZZNNKCAWMIF-UHFFFAOYSA-N
Formula: C22H42O4
SMILES: CCCCCCC(C)OC(=O)C(CC)(CC)C(=O)OC(CCC)C(C)C
Mol. weight [g/mol]: 370.57

Physical Properties

Property code	Value	Unit	Source
gf	-337.96	kJ/mol	Joback Method
hf	-1011.60	kJ/mol	Joback Method
hfus	40.33	kJ/mol	Joback Method
hvap	80.42	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	6.063		Crippen Method
mcvol	335.720	ml/mol	McGowan Method
pc	979.62	kPa	Joback Method
rinpol	2046.00		NIST Webbook
tb	850.79	K	Joback Method
tc	1044.58	K	Joback Method
tf	439.44	K	Joback Method
vc	1.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1093.94	J/mol×K	850.79	Joback Method
cpg	1177.84	J/mol×K	1012.28	Joback Method
cpg	1163.33	J/mol×K	979.98	Joback Method
cpg	1147.73	J/mol×K	947.68	Joback Method
cpg	1130.99	J/mol×K	915.39	Joback Method
cpg	1113.07	J/mol×K	883.09	Joback Method
cpg	1191.28	J/mol×K	1044.58	Joback Method
dvisc	0.0000241	Pa×s	850.79	Joback Method
dvisc	0.0000345	Pa×s	782.23	Joback Method

dvisc	0.0000528	Pa×s	713.67	Joback Method
dvisc	0.0000885	Pa×s	645.12	Joback Method
dvisc	0.0001679	Pa×s	576.56	Joback Method
dvisc	0.0003785	Pa×s	508.00	Joback Method
dvisc	0.0010996	Pa×s	439.44	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369366&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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