Diethylmalonic acid, 2-methylhex-3-yl 4-methylpent-2-yl ester

Inchi: InChI=1S/C20H38O4/c1-9-12-17(15(6)7)24-19(22)20(10-2,11-3)18(21)23-16(8)13-14(4)5

InchiKey: GTSUQJDCGCXONL-UHFFFAOYSA-N

Formula: C20H38O4

SMILES: CCCC(OC(=O)C(CC)(CC)C(=O)OC(C)CC(C)C)C(C)C

Mol. weight [g/mol]: 342.51

Physical Properties

Property code	Value	Unit	Source
gf	-357.24	kJ/mol	Joback Method
hf	-975.60	kJ/mol	Joback Method
hfus	31.62	kJ/mol	Joback Method
hvap	75.58	kJ/mol	Joback Method
log10ws	-5.42		Crippen Method
logp	5.138		Crippen Method
mcvol	307.540	ml/mol	McGowan Method
pc	1114.82	kPa	Joback Method
rinpol	1817.00		NIST Webbook
tb	804.59	K	Joback Method
tc	995.65	K	Joback Method
tf	401.90	K	Joback Method
vc	1.169	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	972.11	J/mol×K	804.59	Joback Method
cpg	990.86	J/mol×K	836.43	Joback Method
cpg	1008.46	J/mol×K	868.28	Joback Method
cpg	1024.95	J/mol×K	900.12	Joback Method
cpg	1040.36	J/mol×K	931.97	Joback Method
cpg	1054.72	J/mol×K	963.81	Joback Method
cpg	1068.06	J/mol×K	995.65	Joback Method
dvisc	0.0019038	Pa×s	401.90	Joback Method
dvisc	0.0005834	Pa×s	469.01	Joback Method

dvisc	0.0002404	Pa×s	536.13	Joback Method
dvisc	0.0001206	Pa×s	603.25	Joback Method
dvisc	0.0000695	Pa×s	670.36	Joback Method
dvisc	0.0000443	Pa×s	737.48	Joback Method
dvisc	0.0000304	Pa×s	804.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370498&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

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