Diethylmalonic acid, isobutyl 3-methylpent-2-yl ester

Inchi: InChI=1S/C17H32O4/c1-8-13(6)14(7)21-16(19)17(9-2,10-3)15(18)20-11-12(4)5/h12-14H

InchiKey: WDNOOMJWNLYHID-UHFFFAOYSA-N

Formula: C17H32O4

SMILES: CCC(C)C(C)OC(=O)C(CC)(CC)C(=O)OCC(C)C

Mol. weight [g/mol]: 300.43

Physical Properties

Property code	Value	Unit	Source
gf	-380.06	kJ/mol	Joback Method
hf	-908.40	kJ/mol	Joback Method
hfus	27.38	kJ/mol	Joback Method
hvap	69.29	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.970		Crippen Method
mcvol	265.270	ml/mol	McGowan Method
pc	1356.63	kPa	Joback Method
rinpol	1643.00		NIST Webbook
tb	736.39	K	Joback Method
tc	924.60	K	Joback Method
tf	383.09	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.31	J/mol×K	736.39	Joback Method
cpg	812.16	J/mol×K	767.76	Joback Method
cpg	829.01	J/mol×K	799.13	Joback Method
cpg	844.86	J/mol×K	830.49	Joback Method
cpg	859.75	J/mol×K	861.86	Joback Method
cpg	873.70	J/mol×K	893.23	Joback Method
cpg	886.74	J/mol×K	924.60	Joback Method
dvisc	0.0022559	Pa×s	383.09	Joback Method
dvisc	0.0007942	Pa×s	441.97	Joback Method

dvisc	0.0003574	Pa×s	500.86	Joback Method
dvisc	0.0001903	Pa×s	559.74	Joback Method
dvisc	0.0001142	Pa×s	618.62	Joback Method
dvisc	0.0000749	Pa×s	677.51	Joback Method
dvisc	0.0000526	Pa×s	736.39	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369728&Units=SI

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