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

Inchi: InChI=1S/C17H32O4/c1-8-17(9-2,14(18)20-10-3)15(19)21-12-13(4)11-16(5,6)7/h13H,8-1

InchiKey: NKOWZVXFTIZKQH-UHFFFAOYSA-N

Formula: C17H32O4

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

Mol. weight [g/mol]: 300.43

Physical Properties

Property code	Value	Unit	Source
gf	-372.34	kJ/mol	Joback Method
hf	-906.59	kJ/mol	Joback Method
hfus	27.01	kJ/mol	Joback Method
hvap	68.77	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.971		Crippen Method
mcvol	265.270	ml/mol	McGowan Method
pc	1359.63	kPa	Joback Method
rinpol	1660.00		NIST Webbook
rinpol	1660.00		NIST Webbook
tb	734.04	K	Joback Method
tc	924.09	K	Joback Method
tf	415.51	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.21	J/mol×K	734.04	Joback Method
cpg	874.07	J/mol×K	892.42	Joback Method
cpg	860.20	J/mol×K	860.74	Joback Method
cpg	845.42	J/mol×K	829.07	Joback Method
cpg	829.69	J/mol×K	797.39	Joback Method
cpg	812.97	J/mol×K	765.72	Joback Method
cpg	887.06	J/mol×K	924.09	Joback Method
dvisc	0.0000511	Pa×s	734.04	Joback Method

dvisc	0.0000715	Pa×s	680.95	Joback Method
dvisc	0.0001060	Pa×s	627.86	Joback Method
dvisc	0.0001689	Pa×s	574.77	Joback Method
dvisc	0.0002958	Pa×s	521.69	Joback Method
dvisc	0.0005884	Pa×s	468.60	Joback Method
dvisc	0.0013952	Pa×s	415.51	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=U369473&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