Diethylmalonic acid, heptyl pentyl ester

Inchi: InChI=1S/C19H36O4/c1-5-9-11-12-14-16-23-18(21)19(7-3,8-4)17(20)22-15-13-10-6-2/h5
InchiKey: QFLFECFAEVSXGQ-UHFFFAOYSA-N
Formula: C19H36O4
SMILES: CCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCCC
Mol. weight [g/mol]: 328.49

Physical Properties

Property code	Value	Unit	Source
gf	-355.90	kJ/mol	Joback Method
hf	-933.84	kJ/mol	Joback Method
hfus	43.13	kJ/mol	Joback Method
hvap	74.90	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	5.040		Crippen Method
mcvol	293.450	ml/mol	McGowan Method
pc	1164.04	kPa	Joback Method
rinpol	1965.00		NIST Webbook
rinpol	1965.00		NIST Webbook
tb	783.47	K	Joback Method
tc	967.35	K	Joback Method
tf	450.63	K	Joback Method
vc	1.137	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	910.17	J/mol×K	783.47	Joback Method
cpg	928.06	J/mol×K	814.12	Joback Method
cpg	944.94	J/mol×K	844.76	Joback Method
cpg	960.85	J/mol×K	875.41	Joback Method
cpg	975.81	J/mol×K	906.05	Joback Method
cpg	989.85	J/mol×K	936.70	Joback Method
cpg	1003.00	J/mol×K	967.35	Joback Method
dvisc	0.0009035	Pa×s	450.63	Joback Method

dvisc	0.0004275	Pa×s	506.10	Joback Method
dvisc	0.0002345	Pa×s	561.58	Joback Method
dvisc	0.0001433	Pa×s	617.05	Joback Method
dvisc	0.0000950	Pa×s	672.52	Joback Method
dvisc	0.0000670	Pa×s	728.00	Joback Method
dvisc	0.0000497	Pa×s	783.47	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=U369515&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

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