

Diethylmalonic acid, hexyl 4-methylpent-2-yl ester

Inchi:	InChI=1S/C19H36O4/c1-7-10-11-12-13-22-17(20)19(8-2,9-3)18(21)23-16(6)14-15(4)5/h1
InchiKey:	QORYBOMZPYQEKU-UHFFFAOYSA-N
Formula:	C19H36O4
SMILES:	CCCCCOC(=O)C(CC)(CC)C(=O)OC(C)CC(C)C
Mol. weight [g/mol]:	328.49

Physical Properties

Property code	Value	Unit	Source
gf	-360.78	kJ/mol	Joback Method
hf	-944.40	kJ/mol	Joback Method
hfus	36.08	kJ/mol	Joback Method
hvap	74.13	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.894		Crippen Method
mcvol	293.450	ml/mol	McGowan Method
pc	1176.85	kPa	Joback Method
rinpol	1842.00		NIST Webbook
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tb	782.59	K	Joback Method
tc	969.42	K	Joback Method
tf	420.63	K	Joback Method
vc	1.125	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	911.15	J/molxK	782.59	Joback Method
cpg	991.84	J/molxK	938.28	Joback Method
cpg	977.69	J/molxK	907.14	Joback Method
cpg	962.57	J/molxK	876.00	Joback Method
cpg	946.47	J/molxK	844.87	Joback Method
cpg	929.33	J/molxK	813.73	Joback Method
cpg	1005.05	J/molxK	969.42	Joback Method
dvisc	0.0000421	Paxs	782.59	Joback Method

dvisc	0.0000589	Paxs	722.26	Joback Method
dvisc	0.0000876	Paxs	661.94	Joback Method
dvisc	0.0001413	Paxs	601.61	Joback Method
dvisc	0.0002533	Paxs	541.28	Joback Method
dvisc	0.0005259	Paxs	480.96	Joback Method
dvisc	0.0013462	Paxs	420.63	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=U370499&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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