

Diethylmalonic acid, pentyl 1-tert-butyloxyprop-2-yl ester

Inchi:	InChI=1S/C19H36O5/c1-8-11-12-13-22-16(20)19(9-2,10-3)17(21)24-15(4)14-23-18(5,6)7
InchiKey:	PMZGGLLJRBWUPX-UHFFFAOYSA-N
Formula:	C19H36O5
SMILES:	CCCCCOC(=O)C(CC)(CC)C(=O)OC(C)COC(C)(C)C
Mol. weight [g/mol]:	344.49

Physical Properties

Property code	Value	Unit	Source
gf	-460.50	kJ/mol	Joback Method
hf	-1080.09	kJ/mol	Joback Method
hfus	33.38	kJ/mol	Joback Method
hvap	75.63	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	4.273		Crippen Method
mcvol	299.320	ml/mol	McGowan Method
pc	1172.03	kPa	Joback Method
rinsol	1899.00		NIST Webbook
tb	802.22	K	Joback Method
tc	993.19	K	Joback Method
tf	460.28	K	Joback Method
vc	1.137	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	942.97	J/molxK	802.22	Joback Method
cpg	1021.36	J/molxK	961.36	Joback Method
cpg	1007.76	J/molxK	929.53	Joback Method
cpg	993.15	J/molxK	897.70	Joback Method
cpg	977.51	J/molxK	865.88	Joback Method
cpg	960.79	J/molxK	834.05	Joback Method
cpg	1033.99	J/molxK	993.19	Joback Method
dvisc	0.0000273	Paxs	802.22	Joback Method
dvisc	0.0000380	Paxs	745.23	Joback Method

dvisc	0.0000560	Paxs	688.24	Joback Method
dvisc	0.0000883	Paxs	631.25	Joback Method
dvisc	0.0001525	Paxs	574.26	Joback Method
dvisc	0.0002972	Paxs	517.27	Joback Method
dvisc	0.0006832	Paxs	460.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368396&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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