

Diethylmalonic acid, hexyl 4-methoxyphenyl ester

Inchi:	InChI=1S/C20H30O5/c1-5-8-9-10-15-24-18(21)20(6-2,7-3)19(22)25-17-13-11-16(23-4)12
InchiKey:	OTYOKVLNKNVXFH-UHFFFAOYSA-N
Formula:	C20H30O5
SMILES:	CCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(OC)cc1
Mol. weight [g/mol]:	350.45

Physical Properties

Property code	Value	Unit	Source
gf	-349.70	kJ/mol	Joback Method
hf	-861.64	kJ/mol	Joback Method
hfus	40.56	kJ/mol	Joback Method
hvap	82.48	kJ/mol	Joback Method
log10ws	-5.13		Crippen Method
logp	4.530		Crippen Method
mcvol	289.650	ml/mol	McGowan Method
pc	1343.73	kPa	Joback Method
rinqol	2368.00		NIST Webbook
tb	860.43	K	Joback Method
tc	1066.28	K	Joback Method
tf	523.07	K	Joback Method
vc	1.103	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	907.95	J/molxK	860.43	Joback Method
cpg	974.86	J/molxK	1031.97	Joback Method
cpg	963.80	J/molxK	997.66	Joback Method
cpg	951.60	J/molxK	963.35	Joback Method
cpg	938.25	J/molxK	929.05	Joback Method
cpg	923.71	J/molxK	894.74	Joback Method
cpg	984.83	J/molxK	1066.28	Joback Method
dvisc	0.0000323	Paxs	860.43	Joback Method
dvisc	0.0000421	Paxs	804.20	Joback Method

dvisc	0.0000572	Paxs	747.98	Joback Method
dvisc	0.0000817	Paxs	691.75	Joback Method
dvisc	0.0001242	Paxs	635.52	Joback Method
dvisc	0.0002048	Paxs	579.30	Joback Method
dvisc	0.0003761	Paxs	523.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369841&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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