

Diethylmalonic acid, 3-methylphenyl propyl ester

Inchi:	InChI=1S/C17H24O4/c1-5-11-20-15(18)17(6-2,7-3)16(19)21-14-10-8-9-13(4)12-14/h8-10
InchiKey:	WOIGLKRCTDNHOY-UHFFFAOYSA-N
Formula:	C17H24O4
SMILES:	CCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(C)c1
Mol. weight [g/mol]:	292.37

Physical Properties

Property code	Value	Unit	Source
gf	-269.96	kJ/mol	Joback Method
hf	-667.50	kJ/mol	Joback Method
hfus	31.60	kJ/mol	Joback Method
hvap	73.39	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	3.660		Crippen Method
mcvol	241.510	ml/mol	McGowan Method
pc	1703.31	kPa	Joback Method
rinpola	1869.00		NIST Webbook
rinpola	1869.00		NIST Webbook
tb	769.37	K	Joback Method
tc	977.67	K	Joback Method
tf	467.03	K	Joback Method
vc	0.916	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.20	J/molxK	769.37	Joback Method
cpg	721.92	J/molxK	804.09	Joback Method
cpg	736.56	J/molxK	838.80	Joback Method
cpg	750.15	J/molxK	873.52	Joback Method
cpg	762.72	J/molxK	908.23	Joback Method
cpg	774.31	J/molxK	942.95	Joback Method
cpg	784.95	J/molxK	977.67	Joback Method
dvisc	0.0007474	Paxs	467.03	Joback Method

dvisc	0.0004108	Paxs	517.42	Joback Method
dvisc	0.0002511	Paxs	567.81	Joback Method
dvisc	0.0001663	Paxs	618.20	Joback Method
dvisc	0.0001172	Paxs	668.59	Joback Method
dvisc	0.0000867	Paxs	718.98	Joback Method
dvisc	0.0000668	Paxs	769.37	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370010&Units=SI

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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