

Dimethylmalonic acid, di(3-ethylphenyl) ester

Inchi:	InChI=1S/C21H24O4/c1-5-15-9-7-11-17(13-15)24-19(22)21(3,4)20(23)25-18-12-8-10-16
InchiKey:	GMAPRVCHACBOPH-UHFFFAOYSA-N
Formula:	C21H24O4
SMILES:	CCc1cccc(OC(=O)C(C)(C)C(=O)Oc2cccc(CC)c2)c1
Mol. weight [g/mol]:	340.41

Physical Properties

Property code	Value	Unit	Source
gf	-133.50	kJ/mol	Joback Method
hf	-525.00	kJ/mol	Joback Method
hfus	35.61	kJ/mol	Joback Method
hvap	85.23	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	4.349		Crippen Method
mvol	274.110	ml/mol	McGowan Method
pc	1611.58	kPa	Joback Method
rinpol	2452.00		NIST Webbook
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tb	892.55	K	Joback Method
tc	1123.35	K	Joback Method
tf	551.05	K	Joback Method
vc	1.032	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.04	J/molxK	892.55	Joback Method
cpg	853.47	J/molxK	931.02	Joback Method
cpg	866.60	J/molxK	969.48	Joback Method
cpg	878.46	J/molxK	1007.95	Joback Method
cpg	889.14	J/molxK	1046.41	Joback Method
cpg	898.69	J/molxK	1084.88	Joback Method
cpg	907.17	J/molxK	1123.35	Joback Method
dvisc	0.0003639	Paxs	551.05	Joback Method

dvisc	0.0002102	Paxs	607.97	Joback Method
dvisc	0.0001334	Paxs	664.88	Joback Method
dvisc	0.0000910	Paxs	721.80	Joback Method
dvisc	0.0000656	Paxs	778.72	Joback Method
dvisc	0.0000495	Paxs	835.63	Joback Method
dvisc	0.0000387	Paxs	892.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363873&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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