

Dimethylmalonic acid, 3-ethylphenyl octyl ester

Inchi:	InChI=1S/C21H32O4/c1-5-7-8-9-10-11-15-24-19(22)21(3,4)20(23)25-18-14-12-13-17(6-2
InchiKey:	WIMJBJUXGACTOL-UHFFFAOYSA-N
Formula:	C21H32O4
SMILES:	CCCCCCCCOC(=O)C(C)(C)C(=O)Oc1cccc(CC)c1
Mol. weight [g/mol]:	348.48

Physical Properties

Property code	Value	Unit	Source
gf	-236.28	kJ/mol	Joback Method
hf	-750.06	kJ/mol	Joback Method
hfus	41.96	kJ/mol	Joback Method
hvap	82.29	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	5.084		Crippen Method
mcvol	297.870	ml/mol	McGowan Method
pc	1269.16	kPa	Joback Method
rinsol	2352.00		NIST Webbook
tb	860.89	K	Joback Method
tc	1066.30	K	Joback Method
tf	512.11	K	Joback Method
vc	1.141	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	937.93	J/molxK	860.89	Joback Method
cpg	954.39	J/molxK	895.13	Joback Method
cpg	969.67	J/molxK	929.36	Joback Method
cpg	983.83	J/molxK	963.60	Joback Method
cpg	996.89	J/molxK	997.83	Joback Method
cpg	1008.90	J/molxK	1032.07	Joback Method
cpg	1019.92	J/molxK	1066.30	Joback Method
dvisc	0.0004882	Paxs	512.11	Joback Method
dvisc	0.0002558	Paxs	570.24	Joback Method

dvisc	0.0001510	Paxs	628.37	Joback Method
dvisc	0.0000975	Paxs	686.50	Joback Method
dvisc	0.0000674	Paxs	744.63	Joback Method
dvisc	0.0000492	Paxs	802.76	Joback Method
dvisc	0.0000374	Paxs	860.89	Joback Method

Sources

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=U363868&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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