

Dimethylmalonic acid, hexyl 3-methylphenyl ester

Inchi:	InChI=1S/C18H26O4/c1-5-6-7-8-12-21-16(19)18(3,4)17(20)22-15-11-9-10-14(2)13-15/h9
InchiKey:	FHWZAORGHGJZPS-UHFFFAOYSA-N
Formula:	C18H26O4
SMILES:	CCCCCOC(=O)C(C)(C)C(=O)Oc1cccc(C)c1
Mol. weight [g/mol]:	306.40

Physical Properties

Property code	Value	Unit	Source
gf	-261.54	kJ/mol	Joback Method
hf	-688.14	kJ/mol	Joback Method
hfus	34.19	kJ/mol	Joback Method
hvap	75.62	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	4.050		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1575.95	kPa	Joback Method
rinpol	2019.00		NIST Webbook
tb	792.25	K	Joback Method
tc	998.90	K	Joback Method
tf	478.30	K	Joback Method
vc	0.973	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.82	J/molxK	792.25	Joback Method
cpg	778.75	J/molxK	826.69	Joback Method
cpg	793.58	J/molxK	861.13	Joback Method
cpg	807.34	J/molxK	895.58	Joback Method
cpg	820.07	J/molxK	930.02	Joback Method
cpg	831.80	J/molxK	964.46	Joback Method
cpg	842.58	J/molxK	998.90	Joback Method
dvisc	0.0006763	Paxs	478.30	Joback Method
dvisc	0.0003670	Paxs	530.62	Joback Method

dvisc	0.0002223	Paxs	582.95	Joback Method
dvisc	0.0001462	Paxs	635.27	Joback Method
dvisc	0.0001025	Paxs	687.60	Joback Method
dvisc	0.0000756	Paxs	739.92	Joback Method
dvisc	0.0000580	Paxs	792.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363614&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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