

Dimethylmalonic acid, pentyl 2-phenethyl ester

Inchi:	InChI=1S/C18H26O4/c1-4-5-9-13-21-16(19)18(2,3)17(20)22-14-12-15-10-7-6-8-11-15/h6
InchiKey:	FBIOGUUGPBOCER-UHFFFAOYSA-N
Formula:	C18H26O4
SMILES:	CCCCCOC(=O)C(C)(C)C(=O)OCCc1ccccc1
Mol. weight [g/mol]:	306.40

Physical Properties

Property code	Value	Unit	Source
gf	-251.91	kJ/mol	Joback Method
hf	-676.67	kJ/mol	Joback Method
hfus	34.58	kJ/mol	Joback Method
hvap	74.95	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.532		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1594.89	kPa	Joback Method
rinpol	2019.00		NIST Webbook
tb	787.27	K	Joback Method
tc	993.13	K	Joback Method
tf	465.78	K	Joback Method
vc	0.973	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	763.54	J/molxK	787.27	Joback Method
cpg	779.58	J/molxK	821.58	Joback Method
cpg	794.50	J/molxK	855.89	Joback Method
cpg	808.35	J/molxK	890.20	Joback Method
cpg	821.17	J/molxK	924.51	Joback Method
cpg	832.99	J/molxK	958.82	Joback Method
cpg	843.88	J/molxK	993.13	Joback Method
dvisc	0.0008118	Paxs	465.78	Joback Method
dvisc	0.0004162	Paxs	519.36	Joback Method

dvisc	0.0002418	Paxs	572.94	Joback Method
dvisc	0.0001542	Paxs	626.52	Joback Method
dvisc	0.0001055	Paxs	680.11	Joback Method
dvisc	0.0000763	Paxs	733.69	Joback Method
dvisc	0.0000577	Paxs	787.27	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=U361617&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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