

Diethylmalonic acid, 3-methylbenzyl propyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C18H26O4/c1-5-11-21-16(19)18(6-2,7-3)17(20)22-13-15-10-8-9-14(4)12-15/h8-17,20-21,22-23H,1H

LFTODDGBJXXCTJ-UHFFFAOYSA-N

C18H26O4

CCCOC(=O)C(CC)(CC)C(=O)OCc1cccc(C)c1

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	-4.50		Crippen Method
logp	3.798		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1575.95	kPa	Joback Method
rinpol	1978.00		NIST Webbook
tb	792.25	K	Joback Method
tc	998.90	K	Joback Method
tf	478.30	K	Joback Method
vc	0.973	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0002223	Pa×s	582.95	Joback Method
dvisc	0.0001462	Pa×s	635.27	Joback Method
dvisc	0.0001025	Pa×s	687.60	Joback Method
dvisc	0.0000756	Pa×s	739.92	Joback Method
dvisc	0.0000580	Pa×s	792.25	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=U369304&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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