Dimethylmalonic acid, 3-ethylphenyl pentyl ester

Inchi: InChI=1S/C18H26O4/c1-5-7-8-12-21-16(19)18(3,4)17(20)22-15-11-9-10-14(6-2)13-15/h9

InchiKey: UZZLPXGJLBQDDS-UHFFFAOYSA-N

Formula: C18H26O4

SMILES: CCCCCOC(=O)C(C)(C)C(=O)Oc1cccc(CC)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	-4.56		Crippen Method
logp	3.914		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1575.95	kPa	Joback Method
rinpol	2076.00		NIST Webbook
rinpol	2076.00		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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U363866&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