

Diethylmalonic acid, 2,3-dimethylphenyl propyl ester

Inchi: InChI=1S/C18H26O4/c1-6-12-21-16(19)18(7-2,8-3)17(20)22-15-11-9-10-13(4)14(15)5/h9-17
InchiKey: JNYRZXYWJMQSEI-UHFFFAOYSA-N
Formula: C18H26O4
SMILES: CCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(C)c1C
Mol. weight [g/mol]: 306.40

Physical Properties

Property code	Value	Unit	Source
gf	-271.17	kJ/mol	Joback Method
hf	-699.61	kJ/mol	Joback Method
hfus	33.80	kJ/mol	Joback Method
hvap	76.28	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	3.968		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1557.35	kPa	Joback Method
rinpol	2027.00		NIST Webbook
tb	797.23	K	Joback Method
tc	1004.68	K	Joback Method
tf	490.82	K	Joback Method
vc	0.973	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.06	J/mol×K	797.23	Joback Method
cpg	830.59	J/mol×K	970.10	Joback Method
cpg	818.95	J/mol×K	935.53	Joback Method
cpg	806.31	J/mol×K	900.95	Joback Method
cpg	792.64	J/mol×K	866.38	Joback Method
cpg	777.90	J/mol×K	831.80	Joback Method
cpg	841.25	J/mol×K	1004.68	Joback Method
dvisc	0.0000584	Pa×s	797.23	Joback Method
dvisc	0.0000749	Pa×s	746.16	Joback Method

dvisc	0.0000999	Pa×s	695.09	Joback Method
dvisc	0.0001392	Pa×s	644.02	Joback Method
dvisc	0.0002055	Pa×s	592.96	Joback Method
dvisc	0.0003266	Pa×s	541.89	Joback Method
dvisc	0.0005714	Pa×s	490.82	Joback Method

Sources

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=U370563&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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