

Diethylmalonic acid, 4-acetylphenyl ethyl ester

Inchi:	InChI=1S/C17H22O5/c1-5-17(6-2,15(19)21-7-3)16(20)22-14-10-8-13(9-11-14)12(4)18/h8
InchiKey:	GRNIXVZNIVYKBO-UHFFFAOYSA-N
Formula:	C17H22O5
SMILES:	CCOC(=O)C(CC)(CC)C(=O)Oc1ccc(C(C)=O)cc1
Mol. weight [g/mol]:	306.35

Physical Properties

Property code	Value	Unit	Source
gf	-398.88	kJ/mol	Joback Method
hf	-780.08	kJ/mol	Joback Method
hfus	33.20	kJ/mol	Joback Method
hvap	80.14	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.164		Crippen Method
mcvol	243.080	ml/mol	McGowan Method
pc	1795.46	kPa	Joback Method
rinsol	2153.00		NIST Webbook
tb	823.24	K	Joback Method
tc	1037.89	K	Joback Method
tf	516.96	K	Joback Method
vc	0.922	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	722.07	J/molxK	823.24	Joback Method
cpg	735.97	J/molxK	859.02	Joback Method
cpg	748.77	J/molxK	894.79	Joback Method
cpg	760.50	J/molxK	930.57	Joback Method
cpg	771.19	J/molxK	966.34	Joback Method
cpg	780.88	J/molxK	1002.12	Joback Method
cpg	789.60	J/molxK	1037.89	Joback Method
dvisc	0.0005988	Paxs	516.96	Joback Method
dvisc	0.0003483	Paxs	568.01	Joback Method

dvisc	0.0002216	Paxs	619.05	Joback Method
dvisc	0.0001510	Paxs	670.10	Joback Method
dvisc	0.0001086	Paxs	721.15	Joback Method
dvisc	0.0000816	Paxs	772.19	Joback Method
dvisc	0.0000636	Paxs	823.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370078&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
mccvol:	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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