

Diethylmalonic acid, 4-acetylphenyl butyl ester

Inchi:	InChI=1S/C19H26O5/c1-5-8-13-23-17(21)19(6-2,7-3)18(22)24-16-11-9-15(10-12-16)14(4
InchiKey:	KOKNKQBDZDTXJR-UHFFFAOYSA-N
Formula:	C19H26O5
SMILES:	CCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(C(C)=O)cc1
Mol. weight [g/mol]:	334.41

Physical Properties

Property code	Value	Unit	Source
gf	-382.04	kJ/mol	Joback Method
hf	-821.36	kJ/mol	Joback Method
hfus	38.38	kJ/mol	Joback Method
hvap	84.59	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	3.944		Crippen Method
mcvol	271.260	ml/mol	McGowan Method
pc	1535.46	kPa	Joback Method
rinpol	2327.00		NIST Webbook
tb	869.00	K	Joback Method
tc	1081.69	K	Joback Method
tf	539.50	K	Joback Method
vc	1.034	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	836.40	J/molxK	869.00	Joback Method
cpg	850.67	J/molxK	904.45	Joback Method
cpg	863.79	J/molxK	939.90	Joback Method
cpg	875.80	J/molxK	975.34	Joback Method
cpg	886.73	J/molxK	1010.79	Joback Method
cpg	896.63	J/molxK	1046.24	Joback Method
cpg	905.54	J/molxK	1081.69	Joback Method
dvisc	0.0004839	Paxs	539.50	Joback Method
dvisc	0.0002747	Paxs	594.42	Joback Method

dvisc	0.0001717	Paxs	649.33	Joback Method
dvisc	0.0001154	Paxs	704.25	Joback Method
dvisc	0.0000822	Paxs	759.17	Joback Method
dvisc	0.0000613	Paxs	814.08	Joback Method
dvisc	0.0000474	Paxs	869.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370081&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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