Diethylmalonic acid, 2-acethylphenyl butyl ester

Inchi: InChI=1S/C19H26O5/c1-5-8-13-23-17(21)19(6-2,7-3)18(22)24-16-12-10-9-11-15(16)14(4

InchiKey: RDCFRMPQDREMAJ-UHFFFAOYSA-N

Formula: C19H26O5

SMILES: CCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1C(C)=O

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	2199.00		NIST Webbook
rinpol	2199.00		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/mol×K	869.00	Joback Method
cpg	850.67	J/mol×K	904.45	Joback Method
cpg	863.79	J/mol×K	939.90	Joback Method
cpg	875.80	J/mol×K	975.34	Joback Method
cpg	886.73	J/mol×K	1010.79	Joback Method
cpg	896.63	J/mol×K	1046.24	Joback Method
cpg	905.54	J/mol×K	1081.69	Joback Method
dvisc	0.0004839	Pa×s	539.50	Joback Method

dvisc	0.0002747	Pa×s	594.42	Joback Method
dvisc	0.0001717	Pa×s	649.33	Joback Method
dvisc	0.0001154	Pa×s	704.25	Joback Method
dvisc	0.0000822	Pa×s	759.17	Joback Method
dvisc	0.0000613	Pa×s	814.08	Joback Method
dvisc	0.0000474	Pa×s	869.00	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=U370099&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