Diethylmalonic acid, 2-acethylphenyl pentyl ester

Inchi: InChI=1S/C20H28O5/c1-5-8-11-14-24-18(22)20(6-2,7-3)19(23)25-17-13-10-9-12-16(17)1

InchiKey: CCDGWULJRMGFBH-UHFFFAOYSA-N

Formula: C20H28O5

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

Mol. weight [g/mol]: 348.43

Physical Properties

Property code	Value	Unit	Source
gf	-373.62	kJ/mol	Joback Method
hf	-842.00	kJ/mol	Joback Method
hfus	40.97	kJ/mol	Joback Method
hvap	86.81	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.334		Crippen Method
mcvol	285.350	ml/mol	McGowan Method
pc	1426.15	kPa	Joback Method
rinpol	2292.00		NIST Webbook
rinpol	2292.00		NIST Webbook
tb	891.88	K	Joback Method
tc	1104.64	K	Joback Method
tf	550.77	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	894.74	J/mol×K	891.88	Joback Method
cpg	955.53	J/mol×K	1069.18	Joback Method
cpg	945.56	J/mol×K	1033.72	Joback Method
cpg	934.54	J/mol×K	998.26	Joback Method
cpg	922.42	J/mol×K	962.80	Joback Method
cpg	909.17	J/mol×K	927.34	Joback Method
cpg	964.49	J/mol×K	1104.64	Joback Method
dvisc	0.0000408	Pa×s	891.88	Joback Method

dvisc	0.0000529	Pa×s	835.03	Joback Method
dvisc	0.0000712	Pa×s	778.18	Joback Method
dvisc	0.0001005	Pa×s	721.33	Joback Method
dvisc	0.0001504	Pa×s	664.47	Joback Method
dvisc	0.0002428	Pa×s	607.62	Joback Method
dvisc	0.0004325	Pa×s	550.77	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=U370100&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