Diethylmalonic acid, 2-acethylphenyl hexyl ester

Inchi: InChI=1S/C21H30O5/c1-5-8-9-12-15-25-19(23)21(6-2,7-3)20(24)26-18-14-11-10-13-17(1

InchiKey: LOWGJNGUFVPJMS-UHFFFAOYSA-N

Formula: C21H30O5

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

Mol. weight [g/mol]: 362.46

Physical Properties

Property code	Value	Unit	Source
gf	-365.20	kJ/mol	Joback Method
hf	-862.64	kJ/mol	Joback Method
hfus	43.56	kJ/mol	Joback Method
hvap	89.04	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	4.724		Crippen Method
mcvol	299.440	ml/mol	McGowan Method
pc	1328.10	kPa	Joback Method
rinpol	2388.00		NIST Webbook
tb	914.76	K	Joback Method
tc	1128.35	K	Joback Method
tf	562.04	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	953.77	J/mol×K	914.76	Joback Method
cpg	968.36	J/mol×K	950.36	Joback Method
cpg	981.74	J/mol×K	985.96	Joback Method
cpg	993.95	J/mol×K	1021.55	Joback Method
cpg	1005.05	J/mol×K	1057.15	Joback Method
cpg	1015.07	J/mol×K	1092.75	Joback Method
cpg	1024.06	J/mol×K	1128.35	Joback Method
dvisc	0.0003852	Pa×s	562.04	Joback Method
dvisc	0.0002138	Pa×s	620.83	Joback Method

dvisc	0.0001314	Pa×s	679.61	Joback Method
dvisc	0.0000873	Pa×s	738.40	Joback Method
dvisc	0.0000616	Pa×s	797.19	Joback Method
dvisc	0.0000456	Pa×s	855.97	Joback Method
dvisc	0.0000351	Pa×s	914.76	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=U370101&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