Sebacic acid, 2-acetylphenyl pentyl ester

Inchi: InChI=1S/C23H34O5/c1-3-4-13-18-27-22(25)16-9-7-5-6-8-10-17-23(26)28-21-15-12-11-1
InchiKey: YAQYTJHYPMUSSF-UHFFFAOYSA-N
Formula: C23H34O5
SMILES: CCCCCOC(=O)CCCCCCCCC(=O)Oc1ccccc1C(C)=O
Mol. weight [g/mol]: 390.51

Physical Properties

Property code	Value	Unit	Source
gf	-351.20	kJ/mol	Joback Method
hf	-895.17	kJ/mol	Joback Method
hfus	56.15	kJ/mol	Joback Method
hvap	94.79	kJ/mol	Joback Method
log10ws	-6.75		Crippen Method
logp	5.649		Crippen Method
mcvol	327.620	ml/mol	McGowan Method
pc	1145.21	kPa	Joback Method
rinpol	2920.00		NIST Webbook
rinpol	2920.00		NIST Webbook
tb	963.75	K	Joback Method
tc	1180.39	K	Joback Method
tf	582.16	K	Joback Method
vc	1.270	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1073.48	J/mol×K	963.75	Joback Method
cpg	1134.27	J/mol×K	1144.29	Joback Method
cpg	1124.75	J/mol×K	1108.18	Joback Method
cpg	1113.95	J/mol×K	1072.07	Joback Method
cpg	1101.83	J/mol×K	1035.96	Joback Method
cpg	1088.36	J/mol×K	999.86	Joback Method
cpg	1142.53	J/mol×K	1180.39	Joback Method
dvisc	0.0000338	Pa×s	963.75	Joback Method

dvisc	0.0000435	Pa×s	900.15	Joback Method
dvisc	0.0000581	Pa×s	836.55	Joback Method
dvisc	0.0000815	Pa×s	772.95	Joback Method
dvisc	0.0001215	Pa×s	709.36	Joback Method
dvisc	0.0001959	Pa×s	645.76	Joback Method
dvisc	0.0003506	Pa×s	582.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354972&Units=SI
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

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