Sebacic acid, 2-acetylphenyl hexyl ester

Inchi: InChI=1S/C24H36O5/c1-3-4-5-14-19-28-23(26)17-10-8-6-7-9-11-18-24(27)29-22-16-13-1
InchiKey: KBEYRQAFLKKBOX-UHFFFAOYSA-N
Formula: C24H36O5
SMILES: CCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccccc1C(C)=O
Mol. weight [g/mol]: 404.54

Physical Properties

Property code	Value	Unit	Source
gf	-342.78	kJ/mol	Joback Method
hf	-915.81	kJ/mol	Joback Method
hfus	58.74	kJ/mol	Joback Method
hvap	97.01	kJ/mol	Joback Method
log10ws	-7.17		Crippen Method
logp	6.039		Crippen Method
mcvol	341.710	ml/mol	McGowan Method
pc	1074.28	kPa	Joback Method
rinpol	3023.00		NIST Webbook
rinpol	3023.00		NIST Webbook
tb	986.63	K	Joback Method
tc	1207.91	K	Joback Method
tf	593.43	K	Joback Method
vc	1.325	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1134.37	J/mol×K	986.63	Joback Method
cpg	1149.44	J/mol×K	1023.51	Joback Method
cpg	1163.03	J/mol×K	1060.39	Joback Method
cpg	1175.18	J/mol×K	1097.27	Joback Method
cpg	1185.94	J/mol×K	1134.15	Joback Method
cpg	1195.35	J/mol×K	1171.03	Joback Method
cpg	1203.45	J/mol×K	1207.91	Joback Method
dvisc	0.0003118	Pa×s	593.43	Joback Method

dvisc	0.0001724	Pa×s	658.96	Joback Method
dvisc	0.0001061	Pa×s	724.50	Joback Method
dvisc	0.0000708	Pa×s	790.03	Joback Method
dvisc	0.0000503	Pa×s	855.56	Joback Method
dvisc	0.0000375	Pa×s	921.10	Joback Method
dvisc	0.0000290	Pa×s	986.63	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=U354974&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