Sebacic acid, 4-acetylphenyl heptyl ester

Inchi: InChI=1S/C25H38O5/c1-3-4-5-10-13-20-29-24(27)14-11-8-6-7-9-12-15-25(28)30-23-18-1
InchiKey: ZVKILJDZMYDHDM-UHFFFAOYSA-N
Formula: C25H38O5
SMILES: CCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(C(C)=O)cc1
Mol. weight [g/mol]: 418.57

Physical Properties

Property code	Value	Unit	Source
gf	-334.36	kJ/mol	Joback Method
hf	-936.45	kJ/mol	Joback Method
hfus	61.33	kJ/mol	Joback Method
hvap	99.24	kJ/mol	Joback Method
log10ws	-7.59		Crippen Method
logp	6.429		Crippen Method
mcvol	355.800	ml/mol	McGowan Method
pc	1009.73	kPa	Joback Method
rinpol	3332.00		NIST Webbook
tb	1009.51	K	Joback Method
tc	1236.49	K	Joback Method
tf	604.70	K	Joback Method
vc	1.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1195.69	J/mol×K	1009.51	Joback Method
cpg	1210.97	J/mol×K	1047.34	Joback Method
cpg	1224.68	J/mol×K	1085.17	Joback Method
cpg	1236.86	J/mol×K	1123.00	Joback Method
cpg	1247.56	J/mol×K	1160.83	Joback Method
cpg	1256.84	J/mol×K	1198.66	Joback Method
cpg	1264.73	J/mol×K	1236.49	Joback Method
dvisc	0.0002765	Pa×s	604.70	Joback Method
dvisc	0.0001514	Pa×s	672.17	Joback Method

dvisc	0.0000925	Pa×s	739.64	Joback Method
dvisc	0.0000614	Pa×s	807.11	Joback Method
dvisc	0.0000434	Pa×s	874.57	Joback Method
dvisc	0.0000322	Pa×s	942.04	Joback Method
dvisc	0.0000249	Pa×s	1009.51	Joback Method

Sources

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=U354967&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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