Sebacic acid, 4-acetylphenyl ethyl ester

Inchi: InChI=1S/C20H28O5/c1-3-24-19(22)10-8-6-4-5-7-9-11-20(23)25-18-14-12-17(13-15-18)1
InchiKey: MTEWKQGQXSYGRG-UHFFFAOYSA-N
Formula: C20H28O5
SMILES: CCOC(=O)CCCCCCCCC(=O)Oc1ccc(C(C)=O)cc1
Mol. weight [g/mol]: 348.43

Physical Properties

Property code	Value	Unit	Source
gf	-376.46	kJ/mol	Joback Method
hf	-833.25	kJ/mol	Joback Method
hfus	48.38	kJ/mol	Joback Method
hvap	88.11	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	4.478		Crippen Method
mcvol	285.350	ml/mol	McGowan Method
pc	1405.90	kPa	Joback Method
rinpol	2799.00		NIST Webbook
tb	895.11	K	Joback Method
tc	1103.51	K	Joback Method
tf	548.35	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	894.02	J/mol×K	895.11	Joback Method
cpg	908.34	J/mol×K	929.84	Joback Method
cpg	921.47	J/mol×K	964.58	Joback Method
cpg	933.41	J/mol×K	999.31	Joback Method
cpg	944.20	J/mol×K	1034.04	Joback Method
cpg	953.87	J/mol×K	1068.77	Joback Method
cpg	962.42	J/mol×K	1103.51	Joback Method
dvisc	0.0004889	Pa×s	548.35	Joback Method
dvisc	0.0002823	Pa×s	606.14	Joback Method

dvisc	0.0001793	Pa×s	663.94	Joback Method
dvisc	0.0001225	Pa×s	721.73	Joback Method
dvisc	0.0000886	Pa×s	779.52	Joback Method
dvisc	0.0000670	Pa×s	837.32	Joback Method
dvisc	0.0000525	Pa×s	895.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354960&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