Sebacic acid, 3,4-dimethylphenyl pentyl ester

Inchi: InChI=1S/C23H36O4/c1-4-5-12-17-26-22(24)13-10-8-6-7-9-11-14-23(25)27-21-16-15-19
InchiKey: JWQYJPJGJFJSRZ-UHFFFAOYSA-N
Formula: C23H36O4
SMILES: CCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(C)c(C)c1
Mol. weight [g/mol]: 376.53

Physical Properties

Property code	Value	Unit	Source
gf	-231.91	kJ/mol	Joback Method
hf	-794.06	kJ/mol	Joback Method
hfus	54.16	kJ/mol	Joback Method
hvap	88.70	kJ/mol	Joback Method
log10ws	-7.04		Crippen Method
logp	6.063		Crippen Method
mcvol	326.050	ml/mol	McGowan Method
pc	1087.06	kPa	Joback Method
rinpol	2903.00		NIST Webbook
tb	914.86	K	Joback Method
tc	1121.86	K	Joback Method
tf	544.75	K	Joback Method
vc	1.264	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1057.52	J/mol×K	914.86	Joback Method
cpg	1128.16	J/mol×K	1087.36	Joback Method
cpg	1116.54	J/mol×K	1052.86	Joback Method
cpg	1103.70	J/mol×K	1018.36	Joback Method
cpg	1089.60	J/mol×K	983.86	Joback Method
cpg	1074.21	J/mol×K	949.36	Joback Method
cpg	1138.58	J/mol×K	1121.86	Joback Method
dvisc	0.0000364	Pa×s	914.86	Joback Method
dvisc	0.0000466	Pa×s	853.17	Joback Method

dvisc	0.0000621	Pa×s	791.49	Joback Method
dvisc	0.0000869	Pa×s	729.80	Joback Method
dvisc	0.0001294	Pa×s	668.12	Joback Method
dvisc	0.0002088	Pa×s	606.43	Joback Method
dvisc	0.0003755	Pa×s	544.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354580&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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