Sebacic acid, 3,4-dimethylphenyl hexyl ester

Inchi: InChI=1S/C24H38O4/c1-4-5-6-13-18-27-23(25)14-11-9-7-8-10-12-15-24(26)28-22-17-16
InchiKey: SOKAOXDRCZKKJD-UHFFFAOYSA-N
Formula: C24H38O4
SMILES: CCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(C)c(C)c1
Mol. weight [g/mol]: 390.56

Physical Properties

Property code	Value	Unit	Source
gf	-223.49	kJ/mol	Joback Method
hf	-814.70	kJ/mol	Joback Method
hfus	56.75	kJ/mol	Joback Method
hvap	90.93	kJ/mol	Joback Method
log10ws	-7.46		Crippen Method
logp	6.453		Crippen Method
mcvol	340.140	ml/mol	McGowan Method
pc	1021.38	kPa	Joback Method
rinpol	3011.00		NIST Webbook
rinpol	3011.00		NIST Webbook
tb	937.74	K	Joback Method
tc	1148.48	K	Joback Method
tf	556.02	K	Joback Method
vc	1.319	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1118.89	J/mol×K	937.74	Joback Method
cpg	1135.82	J/mol×K	972.86	Joback Method
cpg	1151.36	J/mol×K	1007.99	Joback Method
cpg	1165.54	J/mol×K	1043.11	Joback Method
cpg	1178.40	J/mol×K	1078.24	Joback Method
cpg	1189.97	J/mol×K	1113.36	Joback Method
cpg	1200.28	J/mol×K	1148.48	Joback Method
dvisc	0.0003364	Pa×s	556.02	Joback Method

dvisc	0.0001850	Pa×s	619.64	Joback Method
dvisc	0.0001137	Pa×s	683.26	Joback Method
dvisc	0.0000760	Pa×s	746.88	Joback Method
dvisc	0.0000540	Pa×s	810.50	Joback Method
dvisc	0.0000404	Pa×s	874.12	Joback Method
dvisc	0.0000314	Pa×s	937.74	Joback Method

Sources

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=U354582&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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