Sebacic acid, 3,4-dimethylphenyl isohexyl ester

Inchi: InChI=1S/C24H38O4/c1-19(2)12-11-17-27-23(25)13-9-7-5-6-8-10-14-24(26)28-22-16-15

InchiKey: NKXAQIFWSKBQJM-UHFFFAOYSA-N

Formula: C24H38O4

SMILES: Cc1ccc(OC(=O)CCCCCCCCC(=O)OCCCC(C)C)cc1C

Mol. weight [g/mol]: 390.56

Physical Properties

Property code	Value	Unit	Source
gf	-225.93	kJ/mol	Joback Method
hf	-819.98	kJ/mol	Joback Method
hfus	53.23	kJ/mol	Joback Method
hvap	90.54	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	6.309		Crippen Method
mcvol	340.140	ml/mol	McGowan Method
pc	1026.63	kPa	Joback Method
rinpol	2965.00		NIST Webbook
tb	937.30	K	Joback Method
tc	1148.38	K	Joback Method
tf	541.02	K	Joback Method
vc	1.313	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1119.31	J/mol×K	937.30	Joback Method
cpg	1136.23	J/mol×K	972.48	Joback Method
cpg	1151.74	J/mol×K	1007.66	Joback Method
cpg	1165.88	J/mol×K	1042.84	Joback Method
cpg	1178.68	J/mol×K	1078.02	Joback Method
cpg	1190.17	J/mol×K	1113.20	Joback Method
cpg	1200.39	J/mol×K	1148.38	Joback Method
dvisc	0.0003707	Pa×s	541.02	Joback Method
dvisc	0.0001919	Pa×s	607.07	Joback Method

dvisc	0.0001130	Pa×s	673.11	Joback Method
dvisc	0.0000732	Pa×s	739.16	Joback Method
dvisc	0.0000509	Pa×s	805.21	Joback Method
dvisc	0.0000374	Pa×s	871.25	Joback Method
dvisc	0.0000287	Pa×s	937.30	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=U354581&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