Sebacic acid, 2,4-dimethylpent-3-yl hexyl ester

Inchi: InChI=1S/C23H44O4/c1-6-7-8-15-18-26-21(24)16-13-11-9-10-12-14-17-22(25)27-23(19(
InchiKey: DVTFULKVKSXDPW-UHFFFAOYSA-N
Formula: C23H44O4
SMILES: CCCCCCOC(=O)CCCCCCCCC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]: 384.59

Physical Properties

Property code	Value	Unit	Source
gf	-332.38	kJ/mol	Joback Method
hf	-1023.49	kJ/mol	Joback Method
hfus	50.33	kJ/mol	Joback Method
hvap	83.94	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	6.454		Crippen Method
mcvol	349.810	ml/mol	McGowan Method
pc	912.73	kPa	Joback Method
rinpol	2534.00		NIST Webbook
rinpol	2534.00		NIST Webbook
tb	876.90	K	Joback Method
tc	1073.65	K	Joback Method
tf	448.29	K	Joback Method
vc	1.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1155.84	J/mol×K	876.90	Joback Method
cpg	1240.78	J/mol×K	1040.85	Joback Method
cpg	1226.32	J/mol×K	1008.06	Joback Method
cpg	1210.62	J/mol×K	975.27	Joback Method
cpg	1193.66	J/mol×K	942.48	Joback Method
cpg	1175.41	J/mol×K	909.69	Joback Method
cpg	1254.03	J/mol×K	1073.65	Joback Method
dvisc	0.0000262	Pa×s	876.90	Joback Method

dvisc	0.0000367	Pa×s	805.47	Joback Method
dvisc	0.0000548	Pa×s	734.03	Joback Method
dvisc	0.0000894	Pa×s	662.60	Joback Method
dvisc	0.0001639	Pa×s	591.16	Joback Method
dvisc	0.0003551	Pa×s	519.73	Joback Method
dvisc	0.0009847	Pa×s	448.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355429&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