Sebacic acid, 3,3-dimethylbut-2-yl heptyl ester

Inchi: InChI=1S/C23H44O4/c1-6-7-8-13-16-19-26-21(24)17-14-11-9-10-12-15-18-22(25)27-20(
InchiKey: RCEQHCVMPYSOCU-UHFFFAOYSA-N
Formula: C23H44O4
SMILES: CCCCCCCOC(=O)CCCCCCCCC(=O)OC(C)C(C)(C)C
Mol. weight [g/mol]: 384.59

Physical Properties

Property code	Value	Unit	Source
gf	-324.66	kJ/mol	Joback Method
hf	-1021.68	kJ/mol	Joback Method
hfus	49.96	kJ/mol	Joback Method
hvap	83.42	kJ/mol	Joback Method
log10ws	-7.05		Crippen Method
logp	6.599		Crippen Method
mcvol	349.810	ml/mol	McGowan Method
pc	914.39	kPa	Joback Method
rinpol	2552.00		NIST Webbook
tb	874.55	K	Joback Method
tc	1070.98	K	Joback Method
tf	480.71	K	Joback Method
vc	1.355	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1155.24	J/mol×K	874.55	Joback Method
cpg	1174.64	J/mol×K	907.29	Joback Method
cpg	1192.79	J/mol×K	940.03	Joback Method
cpg	1209.75	J/mol×K	972.76	Joback Method
cpg	1225.54	J/mol×K	1005.50	Joback Method
cpg	1240.21	J/mol×K	1038.24	Joback Method
cpg	1253.82	J/mol×K	1070.98	Joback Method
dvisc	0.0006448	Pa×s	480.71	Joback Method
dvisc	0.0002695	Pa×s	546.35	Joback Method

dvisc	0.0001358	Pa×s	611.99	Joback Method
dvisc	0.0000781	Pa×s	677.63	Joback Method
dvisc	0.0000496	Pa×s	743.27	Joback Method
dvisc	0.0000339	Pa×s	808.91	Joback Method
dvisc	0.0000245	Pa×s	874.55	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=U355601&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