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

Inchi: InChI=1S/C22H42O4/c1-18(2)14-13-17-25-20(23)15-11-9-7-8-10-12-16-21(24)26-19(3)22(4,5)6/h18-19H,7-17H2,1-6H3

InchiKey: SJPYFTIATJOJHE-UHFFFAOYSA-N

Formula: C22H42O4

SMILES: CC(C)CCCOC(=O)CCCCCCCCC(=O)OC(C)C(C)(C)C

Mol. weight [g/mol]: 370.57

Physical Properties

Property code	Value	Unit	Source
gf	-335.52	kJ/mol	Joback Method
hf	-1006.32	kJ/mol	Joback Method
hfus	43.85	kJ/mol	Joback Method
hvap	80.81	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	6.064		Crippen Method
mcvol	335.720	ml/mol	McGowan Method
pc	974.73	kPa	Joback Method
rinpol	2418.00		NIST Webbook
rinpol	2418.00		NIST Webbook
tb	851.23	K	Joback Method
tc	1044.28	K	Joback Method
tf	454.44	K	Joback Method
vc	1.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1093.48	J/mol×K	851.23	Joback Method
cpg	1177.25	J/mol×K	1012.11	Joback Method
cpg	1162.73	J/mol×K	979.93	Joback Method
cpg	1147.14	J/mol×K	947.76	Joback Method
cpg	1130.42	J/mol×K	915.58	Joback Method
cpg	1112.55	J/mol×K	883.41	Joback Method
cpg	1190.72	J/mol×K	1044.28	Joback Method
dvisc	0.0000263	Pa×s	851.23	Joback Method

dvisc	0.0000369	Pa×s	785.10	Joback Method
dvisc	0.0000552	Pa×s	718.97	Joback Method
dvisc	0.0000896	Pa×s	652.84	Joback Method
dvisc	0.0001622	Pa×s	586.70	Joback Method
dvisc	0.0003412	Pa×s	520.57	Joback Method
dvisc	0.0008913	Pa×s	454.44	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=U355599&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