Sebacic acid, isobutyl oct-3-en-2-yl ester

Inchi: InChI=1S/C22H40O4/c1-5-6-7-12-15-20(4)26-22(24)17-14-11-9-8-10-13-16-21(23)25-18
InchiKey: LEKBSFFOUJQLPU-NTCAYCPXSA-N
Formula: C22H40O4
SMILES: CCCCC=CC(C)OC(=O)CCCCCCCCC(=O)OCC(C)C
Mol. weight [g/mol]: 368.55

Physical Properties

Property code	Value	Unit	Source
gf	-258.14	kJ/mol	Joback Method
hf	-880.35	kJ/mol	Joback Method
hfus	51.47	kJ/mol	Joback Method
hvap	82.06	kJ/mol	Joback Method
log10ws	-6.48		Crippen Method
logp	5.985		Crippen Method
mcvol	331.420	ml/mol	McGowan Method
pc	995.13	kPa	Joback Method
rinpol	2431.00		NIST Webbook
rinpol	2431.00		NIST Webbook
tb	858.62	K	Joback Method
tc	1052.44	K	Joback Method
tf	446.94	K	Joback Method
vc	1.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1066.75	J/mol×K	858.62	Joback Method
cpg	1085.35	J/mol×K	890.92	Joback Method
cpg	1102.80	J/mol×K	923.23	Joback Method
cpg	1119.14	J/mol×K	955.53	Joback Method
cpg	1134.39	J/mol×K	987.83	Joback Method
cpg	1148.60	J/mol×K	1020.13	Joback Method
cpg	1161.79	J/mol×K	1052.44	Joback Method
dvisc	0.0008719	Pa×s	446.94	Joback Method

dvisc	0.0003392	Pa×s	515.55	Joback Method
dvisc	0.0001647	Pa×s	584.17	Joback Method
dvisc	0.0000931	Pa×s	652.78	Joback Method
dvisc	0.0000587	Pa×s	721.39	Joback Method
dvisc	0.0000401	Pa×s	790.01	Joback Method
dvisc	0.0000291	Pa×s	858.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355835&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