Sebacic acid, isohexyl 4-methylpent-2-yl ester

Inchi: InChI=1S/C22H42O4/c1-18(2)13-12-16-25-21(23)14-10-8-6-7-9-11-15-22(24)26-20(5)17
InchiKey: ZULITQQUUXRNAZ-UHFFFAOYSA-N
Formula: C22H42O4
SMILES: CC(C)CCCOC(=O)CCCCCCCCC(=O)OC(C)CC(C)C
Mol. weight [g/mol]: 370.57

Physical Properties

Property code	Value	Unit	Source
gf	-340.80	kJ/mol	Joback Method
hf	-1002.85	kJ/mol	Joback Method
hfus	47.74	kJ/mol	Joback Method
hvap	81.71	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	6.064		Crippen Method
mcvol	335.720	ml/mol	McGowan Method
pc	968.07	kPa	Joback Method
rinpol	2413.00		NIST Webbook
tb	854.02	K	Joback Method
tc	1046.45	K	Joback Method
tf	437.02	K	Joback Method
vc	1.298	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1093.43	J/mol×K	854.02	Joback Method
cpg	1177.30	J/mol×K	1014.38	Joback Method
cpg	1162.90	J/mol×K	982.31	Joback Method
cpg	1147.34	J/mol×K	950.24	Joback Method
cpg	1130.59	J/mol×K	918.16	Joback Method
cpg	1112.63	J/mol×K	886.09	Joback Method
cpg	1190.56	J/mol×K	1046.45	Joback Method
dvisc	0.0000305	Pa×s	854.02	Joback Method
dvisc	0.0000427	Pa×s	784.52	Joback Method

dvisc	0.0000637	Pa×s	715.02	Joback Method
dvisc	0.0001037	Pa×s	645.52	Joback Method
dvisc	0.0001897	Pa×s	576.02	Joback Method
dvisc	0.0004097	Pa×s	506.52	Joback Method
dvisc	0.0011301	Pa×s	437.02	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=U355352&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