Sebacic acid, isohexyl pent-4-en-2-yl ester

Inchi: InChI=1S/C21H38O4/c1-5-13-19(4)25-21(23)16-11-9-7-6-8-10-15-20(22)24-17-12-14-18
InchiKey: KQUSCIUECLIXIX-UHFFFAOYSA-N
Formula: C21H38O4
SMILES: C=CCC(C)OC(=O)CCCCCCCCC(=O)OCCCC(C)C
Mol. weight [g/mol]: 354.52

Physical Properties

Property code	Value	Unit	Source
gf	-258.94	kJ/mol	Joback Method
hf	-851.50	kJ/mol	Joback Method
hfus	47.39	kJ/mol	Joback Method
hvap	79.21	kJ/mol	Joback Method
log10ws	-6.06		Crippen Method
logp	5.594		Crippen Method
mcvol	317.330	ml/mol	McGowan Method
pc	1051.41	kPa	Joback Method
rinpol	2358.00		NIST Webbook
tb	828.26	K	Joback Method
tc	1016.75	K	Joback Method
tf	438.99	K	Joback Method
vc	1.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1003.75	J/mol×K	828.26	Joback Method
cpg	1021.99	J/mol×K	859.67	Joback Method
cpg	1039.14	J/mol×K	891.09	Joback Method
cpg	1055.20	J/mol×K	922.50	Joback Method
cpg	1070.20	J/mol×K	953.92	Joback Method
cpg	1084.17	J/mol×K	985.33	Joback Method
cpg	1097.13	J/mol×K	1016.75	Joback Method
dvisc	0.0010680	Pa×s	438.99	Joback Method
dvisc	0.0004385	Pa×s	503.87	Joback Method

dvisc	0.0002206	Pa×s	568.75	Joback Method
dvisc	0.0001277	Pa×s	633.62	Joback Method
dvisc	0.0000819	Pa×s	698.50	Joback Method
dvisc	0.0000566	Pa×s	763.38	Joback Method
dvisc	0.0000414	Pa×s	828.26	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U355952&Units=SI

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