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

Inchi: InChI=1S/C21H38O4/c1-4-6-7-14-18-24-20(22)16-12-10-8-9-11-13-17-21(23)25-19(3)15
InchiKey: YLNCBCIEXHVJSO-UHFFFAOYSA-N
Formula: C21H38O4
SMILES: C=CCC(C)OC(=O)CCCCCCCCC(=O)OCCCCCC
Mol. weight [g/mol]: 354.52

Physical Properties

Property code	Value	Unit	Source
gf	-256.50	kJ/mol	Joback Method
hf	-846.22	kJ/mol	Joback Method
hfus	50.92	kJ/mol	Joback Method
hvap	79.59	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	5.739		Crippen Method
mcvol	317.330	ml/mol	McGowan Method
pc	1045.97	kPa	Joback Method
rinpol	2394.00		NIST Webbook
tb	828.70	K	Joback Method
tc	1016.50	K	Joback Method
tf	453.99	K	Joback Method
vc	1.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1003.27	J/mol×K	828.70	Joback Method
cpg	1083.55	J/mol×K	985.20	Joback Method
cpg	1069.57	J/mol×K	953.90	Joback Method
cpg	1054.58	J/mol×K	922.60	Joback Method
cpg	1038.55	J/mol×K	891.30	Joback Method
cpg	1021.45	J/mol×K	860.00	Joback Method
cpg	1096.52	J/mol×K	1016.50	Joback Method
dvisc	0.0000452	Pa×s	828.70	Joback Method
dvisc	0.0000607	Pa×s	766.25	Joback Method

dvisc	0.0000859	Pa×s	703.80	Joback Method
dvisc	0.0001300	Pa×s	641.35	Joback Method
dvisc	0.0002152	Pa×s	578.89	Joback Method
dvisc	0.0004024	Pa×s	516.44	Joback Method
dvisc	0.0008941	Pa×s	453.99	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=U355953&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