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

Inchi: InChI=1S/C23H42O4/c1-4-6-7-8-13-16-20-26-22(24)18-14-11-9-10-12-15-19-23(25)27-2
InchiKey: DLFLHQGTQNSZDZ-UHFFFAOYSA-N
Formula: C23H42O4
SMILES: C=CCC(C)OC(=O)CCCCCCCCC(=O)OCCCCCCCC
Mol. weight [g/mol]: 382.58

Physical Properties

Property code	Value	Unit	Source
gf	-239.66	kJ/mol	Joback Method
hf	-887.50	kJ/mol	Joback Method
hfus	56.10	kJ/mol	Joback Method
hvap	84.05	kJ/mol	Joback Method
log10ws	-7.14		Crippen Method
logp	6.519		Crippen Method
mcvol	345.510	ml/mol	McGowan Method
pc	927.24	kPa	Joback Method
rinpol	2586.00		NIST Webbook
tb	874.46	K	Joback Method
tc	1070.59	K	Joback Method
tf	476.53	K	Joback Method
vc	1.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1126.53	J/mol×K	874.46	Joback Method
cpg	1145.57	J/mol×K	907.15	Joback Method
cpg	1163.37	J/mol×K	939.84	Joback Method
cpg	1179.96	J/mol×K	972.52	Joback Method
cpg	1195.37	J/mol×K	1005.21	Joback Method
cpg	1209.63	J/mol×K	1037.90	Joback Method
cpg	1222.78	J/mol×K	1070.59	Joback Method
dvisc	0.0007041	Pa×s	476.53	Joback Method
dvisc	0.0003111	Pa×s	542.85	Joback Method

dvisc	0.0001643	Pa×s	609.17	Joback Method
dvisc	0.0000983	Pa×s	675.50	Joback Method
dvisc	0.0000645	Pa×s	741.82	Joback Method
dvisc	0.0000453	Pa×s	808.14	Joback Method
dvisc	0.0000336	Pa×s	874.46	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=U355955&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