

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

Inchi:	InChI=1S/C22H40O4/c1-4-6-7-12-15-19-25-21(23)17-13-10-8-9-11-14-18-22(24)26-20(3)
InchiKey:	JOUSBHQMBFKICW-UHFFFAOYSA-N
Formula:	C22H40O4
SMILES:	C=CCC(C)OC(=O)CCCCCCCC(=O)OCCCCCCC
Mol. weight [g/mol]:	368.55

Physical Properties

Property code	Value	Unit	Source
gf	-248.08	kJ/mol	Joback Method
hf	-866.86	kJ/mol	Joback Method
hfus	53.51	kJ/mol	Joback Method
hvap	81.82	kJ/mol	Joback Method
log10ws	-6.72		Crippen Method
logp	6.129		Crippen Method
mcvol	331.420	ml/mol	McGowan Method
pc	983.93	kPa	Joback Method
rinsol	2492.00		NIST Webbook
tb	851.58	K	Joback Method
tc	1043.11	K	Joback Method
tf	465.26	K	Joback Method
vc	1.290	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1064.56	J/molxK	851.58	Joback Method
cpg	1146.23	J/molxK	1011.19	Joback Method
cpg	1132.10	J/molxK	979.27	Joback Method
cpg	1116.90	J/molxK	947.35	Joback Method
cpg	1100.60	J/molxK	915.42	Joback Method
cpg	1083.16	J/molxK	883.50	Joback Method
cpg	1159.30	J/molxK	1043.11	Joback Method
dvisc	0.0000390	Paxs	851.58	Joback Method
dvisc	0.0000525	Paxs	787.19	Joback Method

dvisc	0.0000745	Paxs	722.81	Joback Method
dvisc	0.0001132	Paxs	658.42	Joback Method
dvisc	0.0001883	Paxs	594.03	Joback Method
dvisc	0.0003544	Paxs	529.65	Joback Method
dvisc	0.0007948	Paxs	465.26	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U355954&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

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