

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

Inchi:	InChI=1S/C25H46O4/c1-4-6-7-8-9-12-15-18-22-28-24(26)20-16-13-10-11-14-17-21-25(2
InchiKey:	GZGBCGBMLNAHMY-UHFFFAOYSA-N
Formula:	C25H46O4
SMILES:	C=CCC(C)OC(=O)CCCCCCCCC(=O)OCCCCCCCCC
Mol. weight [g/mol]:	410.63

Physical Properties

Property code	Value	Unit	Source
gf	-222.82	kJ/mol	Joback Method
hf	-928.78	kJ/mol	Joback Method
hfus	61.28	kJ/mol	Joback Method
hvap	88.50	kJ/mol	Joback Method
log10ws	-7.98		Crippen Method
logp	7.299		Crippen Method
mcvol	373.690	ml/mol	McGowan Method
pc	827.64	kPa	Joback Method
rinsol	2772.00		NIST Webbook
tb	920.22	K	Joback Method
tc	1128.41	K	Joback Method
tf	499.07	K	Joback Method
vc	1.458	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1252.27	J/molxK	920.22	Joback Method
cpg	1272.30	J/molxK	954.92	Joback Method
cpg	1290.88	J/molxK	989.62	Joback Method
cpg	1308.06	J/molxK	1024.31	Joback Method
cpg	1323.89	J/molxK	1059.01	Joback Method
cpg	1338.40	J/molxK	1093.71	Joback Method
cpg	1351.64	J/molxK	1128.41	Joback Method
dvisc	0.0005474	Paxs	499.07	Joback Method
dvisc	0.0002378	Paxs	569.26	Joback Method

dvisc	0.0001241	Paxs	639.45	Joback Method
dvisc	0.0000736	Paxs	709.64	Joback Method
dvisc	0.0000480	Paxs	779.84	Joback Method
dvisc	0.0000336	Paxs	850.03	Joback Method
dvisc	0.0000248	Paxs	920.22	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=U355957&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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