

Sebacic acid, heptyl trans-3-hexenyl ester

Inchi:	InChI=1S/C23H42O4/c1-3-5-7-13-17-21-27-23(25)19-15-12-10-9-11-14-18-22(24)26-20-
InchiKey:	NAQLRNNIJULCDL-SOFGYWHQSA-N
Formula:	C23H42O4
SMILES:	CCC=CCCOC(=O)CCCCCCCC(=O)OCCCCCCC
Mol. weight [g/mol]:	382.58

Physical Properties

Property code	Value	Unit	Source
gf	-244.84	kJ/mol	Joback Method
hf	-890.43	kJ/mol	Joback Method
hfus	61.10	kJ/mol	Joback Method
hvap	85.06	kJ/mol	Joback Method
log10ws	-7.03		Crippen Method
logp	6.520		Crippen Method
mcvol	345.510	ml/mol	McGowan Method
pc	928.37	kPa	Joback Method
rinsol	2673.00		NIST Webbook
tb	882.38	K	Joback Method
tc	1080.29	K	Joback Method
tf	488.21	K	Joback Method
vc	1.351	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1127.87	J/molxK	882.38	Joback Method
cpg	1146.91	J/molxK	915.36	Joback Method
cpg	1164.75	J/molxK	948.35	Joback Method
cpg	1181.44	J/molxK	981.33	Joback Method
cpg	1197.00	J/molxK	1014.32	Joback Method
cpg	1211.47	J/molxK	1047.30	Joback Method
cpg	1224.91	J/molxK	1080.29	Joback Method
dvisc	0.0005530	Paxs	488.21	Joback Method
dvisc	0.0002548	Paxs	553.90	Joback Method

dvisc	0.0001384	Paxs	619.60	Joback Method
dvisc	0.0000845	Paxs	685.30	Joback Method
dvisc	0.0000562	Paxs	750.99	Joback Method
dvisc	0.0000400	Paxs	816.68	Joback Method
dvisc	0.0000299	Paxs	882.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356063&Units=SI
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

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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