

Sebacic acid, hexyl pent-4-enyl ester

Inchi:	InChI=1S/C21H38O4/c1-3-5-7-15-19-25-21(23)17-13-11-9-8-10-12-16-20(22)24-18-14-6
InchiKey:	XVIGGHIBKXBZQA-UHFFFAOYSA-N
Formula:	C21H38O4
SMILES:	C=CCCCOC(=O)CCCCCCCC(=O)OCCCCC
Mol. weight [g/mol]:	354.52

Physical Properties

Property code	Value	Unit	Source
gf	-254.06	kJ/mol	Joback Method
hf	-840.94	kJ/mol	Joback Method
hfus	54.44	kJ/mol	Joback Method
hvap	79.98	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	5.740		Crippen Method
mvol	317.330	ml/mol	McGowan Method
pc	1040.58	kPa	Joback Method
rinpol	2488.00		NIST Webbook
rinpol	2488.00		NIST Webbook
tb	829.14	K	Joback Method
tc	1016.39	K	Joback Method
tf	468.99	K	Joback Method
vc	1.240	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1002.79	J/molxK	829.14	Joback Method
cpg	1020.92	J/molxK	860.35	Joback Method
cpg	1037.99	J/molxK	891.56	Joback Method
cpg	1054.00	J/molxK	922.77	Joback Method
cpg	1068.99	J/molxK	953.97	Joback Method
cpg	1082.97	J/molxK	985.18	Joback Method
cpg	1095.98	J/molxK	1016.39	Joback Method
dvisc	0.0007636	Paxs	468.99	Joback Method

dvisc	0.0003732	Paxs	529.01	Joback Method
dvisc	0.0002110	Paxs	589.04	Joback Method
dvisc	0.0001326	Paxs	649.07	Joback Method
dvisc	0.0000902	Paxs	709.09	Joback Method
dvisc	0.0000651	Paxs	769.12	Joback Method
dvisc	0.0000493	Paxs	829.14	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=U355413&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

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