

Sebacic acid, di(pent-4-enyl) ester

Inchi:	InChI=1S/C20H34O4/c1-3-5-13-17-23-19(21)15-11-9-7-8-10-12-16-20(22)24-18-14-6-4-2
InchiKey:	ZZKXHYGNRATKKE-UHFFFAOYSA-N
Formula:	C20H34O4
SMILES:	C=CCCCOC(=O)CCCCCCCCC(=O)OCCCC=C
Mol. weight [g/mol]:	338.48

Physical Properties

Property code	Value	Unit	Source
gf	-174.64	kJ/mol	Joback Method
hf	-694.87	kJ/mol	Joback Method
hfus	50.57	kJ/mol	Joback Method
hvap	77.09	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	5.126		Crippen Method
mvol	298.940	ml/mol	McGowan Method
pc	1139.80	kPa	Joback Method
rinpol	2387.00		NIST Webbook
tb	802.94	K	Joback Method
tc	987.36	K	Joback Method
tf	455.96	K	Joback Method
vc	1.165	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	915.44	J/molxK	802.94	Joback Method
cpg	991.74	J/molxK	956.62	Joback Method
cpg	978.34	J/molxK	925.89	Joback Method
cpg	964.03	J/molxK	895.15	Joback Method
cpg	948.79	J/molxK	864.41	Joback Method
cpg	932.60	J/molxK	833.68	Joback Method
cpg	1004.26	J/molxK	987.36	Joback Method
dvisc	0.0000606	Paxs	802.94	Joback Method
dvisc	0.0000795	Paxs	745.11	Joback Method

dvisc	0.0001091	Paxs	687.28	Joback Method
dvisc	0.0001586	Paxs	629.45	Joback Method
dvisc	0.0002487	Paxs	571.62	Joback Method
dvisc	0.0004316	Paxs	513.79	Joback Method
dvisc	0.0008615	Paxs	455.96	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=U355418&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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