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
mcvol	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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	915.44	J/mol×K	802.94	Joback Method
cpg	932.60	J/mol×K	833.68	Joback Method
cpg	948.79	J/mol×K	864.41	Joback Method
cpg	964.03	J/mol×K	895.15	Joback Method
cpg	978.34	J/mol×K	925.89	Joback Method
cpg	991.74	J/mol×K	956.62	Joback Method
cpg	1004.26	J/mol×K	987.36	Joback Method
dvisc	0.0008615	Pa×s	455.96	Joback Method
dvisc	0.0004316	Pa×s	513.79	Joback Method

dvisc	0.0002487	Pa×s	571.62	Joback Method
dvisc	0.0001586	Pa×s	629.45	Joback Method
dvisc	0.0001091	Pa×s	687.28	Joback Method
dvisc	0.0000795	Pa×s	745.11	Joback Method
dvisc	0.0000606	Pa×s	802.94	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/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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