

Sebacic acid, but-3-enyl pentyl ester

Inchi:	InChI=1S/C19H34O4/c1-3-5-13-17-23-19(21)15-12-10-8-7-9-11-14-18(20)22-16-6-4-2/h4
InchiKey:	UPVFJMDNNUJSQE-UHFFFAOYSA-N
Formula:	C19H34O4
SMILES:	C=CCCOC(=O)CCCCCCCCC(=O)OCCCCC
Mol. weight [g/mol]:	326.47

Physical Properties

Property code	Value	Unit	Source
gf	-270.90	kJ/mol	Joback Method
hf	-799.66	kJ/mol	Joback Method
hfus	49.26	kJ/mol	Joback Method
hvap	75.53	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.960		Crippen Method
mcvol	289.150	ml/mol	McGowan Method
pc	1182.53	kPa	Joback Method
rinpol	2274.00		NIST Webbook
rinpol	2274.00		NIST Webbook
tb	783.38	K	Joback Method
tc	964.87	K	Joback Method
tf	446.45	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	882.52	J/mol×K	783.38	Joback Method
cpg	959.66	J/mol×K	934.62	Joback Method
cpg	946.06	J/mol×K	904.37	Joback Method
cpg	931.56	J/mol×K	874.12	Joback Method
cpg	916.15	J/mol×K	843.88	Joback Method
cpg	899.80	J/mol×K	813.63	Joback Method
cpg	972.38	J/mol×K	964.87	Joback Method
dvisc	0.0000654	Pa×s	783.38	Joback Method

dvisc	0.0000860	Pa×s	727.23	Joback Method
dvisc	0.0001183	Pa×s	671.07	Joback Method
dvisc	0.0001724	Pa×s	614.92	Joback Method
dvisc	0.0002712	Pa×s	558.76	Joback Method
dvisc	0.0004720	Pa×s	502.61	Joback Method
dvisc	0.0009442	Pa×s	446.45	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=U356084&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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