

Sebacic acid, but-3-enyl hexyl ester

Inchi:	InChI=1S/C20H36O4/c1-3-5-7-14-18-24-20(22)16-13-11-9-8-10-12-15-19(21)23-17-6-4-2
InchiKey:	IDMMLLXRKDEBJO-UHFFFAOYSA-N
Formula:	C20H36O4
SMILES:	C=CCCOC(=O)CCCCCCCC(=O)OCCCCC
Mol. weight [g/mol]:	340.50

Physical Properties

Property code	Value	Unit	Source
gf	-262.48	kJ/mol	Joback Method
hf	-820.30	kJ/mol	Joback Method
hfus	51.85	kJ/mol	Joback Method
hvap	77.76	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	5.350		Crippen Method
mvol	303.240	ml/mol	McGowan Method
pc	1108.15	kPa	Joback Method
rinpol	2373.00		NIST Webbook
tb	806.26	K	Joback Method
tc	990.25	K	Joback Method
tf	457.72	K	Joback Method
vc	1.185	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	942.24	J/molxK	806.26	Joback Method
cpg	1020.90	J/molxK	959.59	Joback Method
cpg	1007.10	J/molxK	928.92	Joback Method
cpg	992.36	J/molxK	898.26	Joback Method
cpg	976.64	J/molxK	867.59	Joback Method
cpg	959.95	J/molxK	836.93	Joback Method
cpg	1033.77	J/molxK	990.25	Joback Method
dvisc	0.0000569	Paxs	806.26	Joback Method
dvisc	0.0000749	Paxs	748.17	Joback Method

dvisc	0.0001034	Paxs	690.08	Joback Method
dvisc	0.0001515	Paxs	631.99	Joback Method
dvisc	0.0002396	Paxs	573.90	Joback Method
dvisc	0.0004205	Paxs	515.81	Joback Method
dvisc	0.0008509	Paxs	457.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356086&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

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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