

Sebacic acid, dodecyl 6-ethyloct-3-yl ester

Inchi:	InChI=1S/C32H62O4/c1-5-9-10-11-12-13-14-17-20-23-28-35-31(33)24-21-18-15-16-19-2
InchiKey:	ODIHBPOXKAJDCZ-UHFFFAOYSA-N
Formula:	C32H62O4
SMILES:	CCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OC(CC)CCC(CC)CC
Mol. weight [g/mol]:	510.83

Physical Properties

Property code	Value	Unit	Source
gf	-254.16	kJ/mol	Joback Method
hf	-1203.97	kJ/mol	Joback Method
hfus	77.16	kJ/mol	Joback Method
hvap	104.36	kJ/mol	Joback Method
log10ws	-10.81		Crippen Method
logp	10.109		Crippen Method
mvol	476.620	ml/mol	McGowan Method
pc	571.78	kPa	Joback Method
rinpol	3461.00		NIST Webbook
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tb	1083.26	K	Joback Method
tc	1374.80	K	Joback Method
tf	564.72	K	Joback Method
vc	1.863	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1736.98	J/molxK	1083.26	Joback Method
cpg	1833.76	J/molxK	1326.21	Joback Method
cpg	1819.84	J/molxK	1277.62	Joback Method
cpg	1803.37	J/molxK	1229.03	Joback Method
cpg	1784.18	J/molxK	1180.44	Joback Method
cpg	1762.10	J/molxK	1131.85	Joback Method
cpg	1845.29	J/molxK	1374.80	Joback Method
dvisc	0.0000068	Paxs	1083.26	Joback Method

dvisc	0.0000095	Paxs	996.84	Joback Method
dvisc	0.0000140	Paxs	910.41	Joback Method
dvisc	0.0000226	Paxs	823.99	Joback Method
dvisc	0.0000407	Paxs	737.57	Joback Method
dvisc	0.0000857	Paxs	651.14	Joback Method
dvisc	0.0002266	Paxs	564.72	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354193&Units=SI

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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