

Sebacic acid, 5-methoxy-3-methylpentyl tridecyl ester

Inchi:	InChI=1S/C30H58O5/c1-4-5-6-7-8-9-10-11-14-17-20-25-34-29(31)21-18-15-12-13-16-19
InchiKey:	KGKUYFURLXVZIL-UHFFFAOYSA-N
Formula:	C30H58O5
SMILES:	CCCCCCCCCCCCOC(=O)CCCCCCCC(=O)OCCC(C)CCOC
Mol. weight [g/mol]:	498.78

Physical Properties

Property code	Value	Unit	Source
gf	-373.56	kJ/mol	Joback Method
hf	-1289.63	kJ/mol	Joback Method
hfus	76.69	kJ/mol	Joback Method
hvap	102.71	kJ/mol	Joback Method
log10ws	-8.95		Crippen Method
logp	8.567		Crippen Method
mcvol	454.310	ml/mol	McGowan Method
pc	620.34	kPa	Joback Method
rinpol	3470.00		NIST Webbook
rinpol	3470.00		NIST Webbook
tb	1060.36	K	Joback Method
tc	1338.15	K	Joback Method
tf	579.41	K	Joback Method
vc	1.776	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1635.89	J/molxK	1060.36	Joback Method
cpg	1722.21	J/molxK	1291.85	Joback Method
cpg	1710.56	J/molxK	1245.55	Joback Method
cpg	1696.21	J/molxK	1199.25	Joback Method
cpg	1679.04	J/molxK	1152.96	Joback Method
cpg	1658.96	J/molxK	1106.66	Joback Method
cpg	1731.24	J/molxK	1338.15	Joback Method
dvisc	0.0000076	Paxs	1060.36	Joback Method

dvisc	0.0000103	Paxs	980.20	Joback Method
dvisc	0.0000149	Paxs	900.04	Joback Method
dvisc	0.0000231	Paxs	819.88	Joback Method
dvisc	0.0000393	Paxs	739.73	Joback Method
dvisc	0.0000763	Paxs	659.57	Joback Method
dvisc	0.0001777	Paxs	579.41	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=U355511&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
log_p:	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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