

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

Inchi:	InChI=1S/C28H54O5/c1-4-5-6-7-8-9-12-15-18-23-32-27(29)19-16-13-10-11-14-17-20-28
InchiKey:	MTLINFLFZDWHQR-UHFFFAOYSA-N
Formula:	C28H54O5
SMILES:	CCCCCCCCCOC(=O)CCCCCCCC(=O)OCCC(C)CCOC
Mol. weight [g/mol]:	470.73

Physical Properties

Property code	Value	Unit	Source
gf	-390.40	kJ/mol	Joback Method
hf	-1248.35	kJ/mol	Joback Method
hfus	71.52	kJ/mol	Joback Method
hvap	98.26	kJ/mol	Joback Method
log10ws	-8.11		Crippen Method
logp	7.787		Crippen Method
mcvol	426.130	ml/mol	McGowan Method
pc	684.21	kPa	Joback Method
rinsol	3255.00		NIST Webbook
tb	1014.60	K	Joback Method
tc	1263.85	K	Joback Method
tf	556.87	K	Joback Method
vc	1.663	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1506.22	J/molxK	1014.60	Joback Method
cpg	1528.11	J/molxK	1056.14	Joback Method
cpg	1547.60	J/molxK	1097.68	Joback Method
cpg	1564.77	J/molxK	1139.22	Joback Method
cpg	1579.67	J/molxK	1180.76	Joback Method
cpg	1592.37	J/molxK	1222.30	Joback Method
cpg	1602.91	J/molxK	1263.85	Joback Method
dvisc	0.0002359	Paxs	556.87	Joback Method
dvisc	0.0001027	Paxs	633.16	Joback Method

dvisc	0.0000535	Paxs	709.45	Joback Method
dvisc	0.0000316	Paxs	785.73	Joback Method
dvisc	0.0000205	Paxs	862.02	Joback Method
dvisc	0.0000143	Paxs	938.31	Joback Method
dvisc	0.0000105	Paxs	1014.60	Joback Method

Sources

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=U355509&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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