

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

Inchi:	InChI=1S/C25H48O5/c1-4-5-6-7-12-15-20-29-24(26)16-13-10-8-9-11-14-17-25(27)30-22
InchiKey:	WBEFLJUIOHSEJN-UHFFFAOYSA-N
Formula:	C25H48O5
SMILES:	CCCCCCCCOC(=O)CCCCCCCC(=O)OCCC(C)CCOC
Mol. weight [g/mol]:	428.65

Physical Properties

Property code	Value	Unit	Source
gf	-415.66	kJ/mol	Joback Method
hf	-1186.43	kJ/mol	Joback Method
hfus	63.74	kJ/mol	Joback Method
hvap	91.58	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	6.617		Crippen Method
mvol	383.860	ml/mol	McGowan Method
pc	800.24	kPa	Joback Method
rinpol	2968.00		NIST Webbook
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tb	945.96	K	Joback Method
tc	1163.54	K	Joback Method
tf	523.06	K	Joback Method
vc	1.496	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1313.62	J/molxK	945.96	Joback Method
cpg	1397.77	J/molxK	1127.28	Joback Method
cpg	1384.32	J/molxK	1091.02	Joback Method
cpg	1369.21	J/molxK	1054.75	Joback Method
cpg	1352.40	J/molxK	1018.49	Joback Method
cpg	1333.88	J/molxK	982.22	Joback Method
cpg	1409.59	J/molxK	1163.54	Joback Method
dvisc	0.0000169	Paxs	945.96	Joback Method

dvisc	0.0000229	Paxs	875.48	Joback Method
dvisc	0.0000327	Paxs	804.99	Joback Method
dvisc	0.0000501	Paxs	734.51	Joback Method
dvisc	0.0000837	Paxs	664.03	Joback Method
dvisc	0.0001583	Paxs	593.54	Joback Method
dvisc	0.0003553	Paxs	523.06	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=U355506&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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