

Sebacic acid, 5-methoxy-3-phenylpentyl propyl ester

Inchi:	InChI=1S/C25H40O5/c1-3-19-29-24(26)15-11-6-4-5-7-12-16-25(27)30-21-18-23(17-20-2
InchiKey:	ZMDZYMJUTUZUCP-UHFFFAOYSA-N
Formula:	C25H40O5
SMILES:	CCCOC(=O)CCCCCCCCC(=O)OCCC(CCOC)c1ccccc1
Mol. weight [g/mol]:	420.58

Physical Properties

Property code	Value	Unit	Source
gf	-303.25	kJ/mol	Joback Method
hf	-949.90	kJ/mol	Joback Method
hfus	57.79	kJ/mol	Joback Method
hvap	93.85	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	5.814		Crippen Method
mcvol	360.100	ml/mol	McGowan Method
pc	974.13	kPa	Joback Method
rinpol	2990.00		NIST Webbook
tb	972.64	K	Joback Method
tc	1190.89	K	Joback Method
tf	549.48	K	Joback Method
vc	1.387	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1211.98	J/molxK	972.64	Joback Method
cpg	1228.63	J/molxK	1009.01	Joback Method
cpg	1243.66	J/molxK	1045.39	Joback Method
cpg	1257.11	J/molxK	1081.76	Joback Method
cpg	1269.03	J/molxK	1118.14	Joback Method
cpg	1279.44	J/molxK	1154.51	Joback Method
cpg	1288.38	J/molxK	1190.89	Joback Method
dvisc	0.0002999	Paxs	549.48	Joback Method
dvisc	0.0001425	Paxs	620.01	Joback Method

dvisc	0.0000788	Paxs	690.53	Joback Method
dvisc	0.0000487	Paxs	761.06	Joback Method
dvisc	0.0000326	Paxs	831.59	Joback Method
dvisc	0.0000233	Paxs	902.11	Joback Method
dvisc	0.0000174	Paxs	972.64	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=U355480&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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