

Sebacic acid, hexyl 4-methoxy-2-methylbutyl ester

Other names:	Sebacic acid, hexyl 4-methoxy-2-methylphenyl ester
Inchi:	InChI=1S/C22H42O5/c1-4-5-6-13-17-26-21(23)14-11-9-7-8-10-12-15-22(24)27-19-20(2)
InchiKey:	XCWRHNAFSITOJZ-UHFFFAOYSA-N
Formula:	C22H42O5
SMILES:	CCCCCOC(=O)CCCCCCCC(=O)OCC(C)CCOC
Mol. weight [g/mol]:	386.57

Physical Properties

Property code	Value	Unit	Source
gf	-440.92	kJ/mol	Joback Method
hf	-1124.51	kJ/mol	Joback Method
hfus	55.97	kJ/mol	Joback Method
hvap	84.90	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	5.447		Crippen Method
mcvol	341.590	ml/mol	McGowan Method
pc	948.50	kPa	Joback Method
rinpol	2652.00		NIST Webbook
tb	877.32	K	Joback Method
tc	1074.12	K	Joback Method
tf	489.25	K	Joback Method
vc	1.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1124.56	J/molxK	877.32	Joback Method
cpg	1143.45	J/molxK	910.12	Joback Method
cpg	1161.00	J/molxK	942.92	Joback Method
cpg	1177.23	J/molxK	975.72	Joback Method
cpg	1192.16	J/molxK	1008.52	Joback Method
cpg	1205.79	J/molxK	1041.32	Joback Method
cpg	1218.14	J/molxK	1074.12	Joback Method
dvisc	0.0005231	Paxs	489.25	Joback Method

dvisc	0.0002392	Paxs	553.93	Joback Method
dvisc	0.0001288	Paxs	618.61	Joback Method
dvisc	0.0000780	Paxs	683.28	Joback Method
dvisc	0.0000515	Paxs	747.96	Joback Method
dvisc	0.0000363	Paxs	812.64	Joback Method
dvisc	0.0000270	Paxs	877.32	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=U355326&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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