

Sebacic acid, di(4-methoxy-2-methylbutyl) ester

Other names:	Sebacic acid, di(4-methoxy-2-methylphenyl) ester
Inchi:	InChI=1S/C22H42O6/c1-19(13-15-25-3)17-27-21(23)11-9-7-5-6-8-10-12-22(24)28-18-20
InchiKey:	AEDKNRPYRNCPLZ-UHFFFAOYSA-N
Formula:	C22H42O6
SMILES:	COCCC(C)COC(=O)CCCCCCCCC(=O)OCC(C)CCOC
Mol. weight [g/mol]:	402.57

Physical Properties

Property code	Value	Unit	Source
gf	-548.36	kJ/mol	Joback Method
hf	-1262.01	kJ/mol	Joback Method
hfus	53.64	kJ/mol	Joback Method
hvap	86.92	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	4.539		Crippen Method
mcvol	347.460	ml/mol	McGowan Method
pc	943.26	kPa	Joback Method
rinpol	2734.00		NIST Webbook
tb	899.30	K	Joback Method
tc	1101.28	K	Joback Method
tf	496.48	K	Joback Method
vc	1.339	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1156.64	J/molxK	899.30	Joback Method
cpg	1234.03	J/molxK	1067.62	Joback Method
cpg	1221.55	J/molxK	1033.95	Joback Method
cpg	1207.57	J/molxK	1000.29	Joback Method
cpg	1192.09	J/molxK	966.63	Joback Method
cpg	1175.12	J/molxK	932.96	Joback Method
cpg	1245.02	J/molxK	1101.28	Joback Method
dvisc	0.0000182	Paxs	899.30	Joback Method

dvisc	0.0000248	Paxs	832.16	Joback Method
dvisc	0.0000357	Paxs	765.03	Joback Method
dvisc	0.0000549	Paxs	697.89	Joback Method
dvisc	0.0000928	Paxs	630.75	Joback Method
dvisc	0.0001777	Paxs	563.62	Joback Method
dvisc	0.0004054	Paxs	496.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355336&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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