

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

Other names:	Sebacic acid, 4-methoxy-2-methylphenyl pentyl ester
Inchi:	InChI=1S/C21H40O5/c1-4-5-12-16-25-20(22)13-10-8-6-7-9-11-14-21(23)26-18-19(2)15-
InchiKey:	YEOSWXMPRWZYGK-UHFFFAOYSA-N
Formula:	C21H40O5
SMILES:	CCCCCOC(=O)CCCCCCCC(=O)OCC(C)CCOC
Mol. weight [g/mol]:	372.54

Physical Properties

Property code	Value	Unit	Source
gf	-449.34	kJ/mol	Joback Method
hf	-1103.87	kJ/mol	Joback Method
hfus	53.38	kJ/mol	Joback Method
hvap	82.67	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	5.056		Crippen Method
mcvol	327.500	ml/mol	McGowan Method
pc	1007.17	kPa	Joback Method
rinpol	2559.00		NIST Webbook
tb	854.44	K	Joback Method
tc	1046.32	K	Joback Method
tf	477.98	K	Joback Method
vc	1.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1062.62	J/molxK	854.44	Joback Method
cpg	1142.77	J/molxK	1014.34	Joback Method
cpg	1129.16	J/molxK	982.36	Joback Method
cpg	1114.36	J/molxK	950.38	Joback Method
cpg	1098.34	J/molxK	918.40	Joback Method
cpg	1081.09	J/molxK	886.42	Joback Method
cpg	1155.19	J/molxK	1046.32	Joback Method
dvisc	0.0000314	Paxs	854.44	Joback Method

dvisc	0.0000422	Paxs	791.70	Joback Method
dvisc	0.0000597	Paxs	728.95	Joback Method
dvisc	0.0000901	Paxs	666.21	Joback Method
dvisc	0.0001480	Paxs	603.47	Joback Method
dvisc	0.0002731	Paxs	540.72	Joback Method
dvisc	0.0005916	Paxs	477.98	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=U355324&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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