

Sebacic acid, 2,6-dimethoxyphenyl heptyl ester

Inchi:	InChI=1S/C25H40O6/c1-4-5-6-11-14-20-30-23(26)18-12-9-7-8-10-13-19-24(27)31-25-21
InchiKey:	GSBHLIQGWQDJKJ-UHFFFAOYSA-N
Formula:	C25H40O6
SMILES:	CCCCCCCOC(=O)CCCCCCCC(=O)Oc1c(OC)cccc1OC
Mol. weight [g/mol]:	436.58

Physical Properties

Property code	Value	Unit	Source
gf	-425.07	kJ/mol	Joback Method
hf	-1099.78	kJ/mol	Joback Method
hfus	61.72	kJ/mol	Joback Method
hvap	97.98	kJ/mol	Joback Method
log10ws	-7.17		Crippen Method
logp	6.244		Crippen Method
mvol	365.970	ml/mol	McGowan Method
pc	941.52	kPa	Joback Method
rinpol	3252.00		NIST Webbook
tb	1005.46	K	Joback Method
tc	1232.82	K	Joback Method
tf	611.75	K	Joback Method
vc	1.411	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1238.93	J/molxK	1005.46	Joback Method
cpg	1254.45	J/molxK	1043.35	Joback Method
cpg	1268.02	J/molxK	1081.25	Joback Method
cpg	1279.67	J/molxK	1119.14	Joback Method
cpg	1289.40	J/molxK	1157.04	Joback Method
cpg	1297.22	J/molxK	1194.93	Joback Method
cpg	1303.13	J/molxK	1232.82	Joback Method
dvisc	0.0001456	Paxs	611.75	Joback Method
dvisc	0.0000827	Paxs	677.37	Joback Method

dvisc	0.0000519	Paxs	742.99	Joback Method
dvisc	0.0000351	Paxs	808.61	Joback Method
dvisc	0.0000252	Paxs	874.22	Joback Method
dvisc	0.0000189	Paxs	939.84	Joback Method
dvisc	0.0000148	Paxs	1005.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354755&Units=SI
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

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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