

Sebacic acid, heptyl 4-methoxyphenyl ester

Inchi:	InChI=1S/C24H38O5/c1-3-4-5-10-13-20-28-23(25)14-11-8-6-7-9-12-15-24(26)29-22-18-
InchiKey:	HHGADISQVDADAL-UHFFFAOYSA-N
Formula:	C24H38O5
SMILES:	CCCCCCCOC(=O)CCCCCCCC(=O)Oc1ccc(OC)cc1
Mol. weight [g/mol]:	406.56

Physical Properties

Property code	Value	Unit	Source
gf	-318.86	kJ/mol	Joback Method
hf	-935.45	kJ/mol	Joback Method
hfus	58.33	kJ/mol	Joback Method
hvap	92.68	kJ/mol	Joback Method
log10ws	-7.05		Crippen Method
logp	6.235		Crippen Method
mvol	346.010	ml/mol	McGowan Method
pc	1020.08	kPa	Joback Method
rinpol	3147.00		NIST Webbook
rinpol	3147.00		NIST Webbook
tb	955.18	K	Joback Method
tc	1169.41	K	Joback Method
tf	565.73	K	Joback Method
vc	1.337	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1149.17	J/molxK	955.18	Joback Method
cpg	1165.55	J/molxK	990.89	Joback Method
cpg	1180.40	J/molxK	1026.59	Joback Method
cpg	1193.74	J/molxK	1062.30	Joback Method
cpg	1205.60	J/molxK	1098.00	Joback Method
cpg	1216.01	J/molxK	1133.71	Joback Method
cpg	1224.99	J/molxK	1169.41	Joback Method
dvisc	0.0002663	Paxs	565.73	Joback Method

dvisc	0.0001432	Paxs	630.64	Joback Method
dvisc	0.0000864	Paxs	695.55	Joback Method
dvisc	0.0000569	Paxs	760.45	Joback Method
dvisc	0.0000400	Paxs	825.36	Joback Method
dvisc	0.0000296	Paxs	890.27	Joback Method
dvisc	0.0000228	Paxs	955.18	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=U354778&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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