

Sebacic acid, 3-phenylpropyl pentyl ester

Inchi:	InChI=1S/C24H38O4/c1-2-3-13-20-27-23(25)18-11-6-4-5-7-12-19-24(26)28-21-14-17-22
InchiKey:	ZRNNZRWMEVEPRG-UHFFFAOYSA-N
Formula:	C24H38O4
SMILES:	CCCCCOC(=O)CCCCCCCC(=O)OCCc1ccccc1
Mol. weight [g/mol]:	390.56

Physical Properties

Property code	Value	Unit	Source
gf	-204.23	kJ/mol	Joback Method
hf	-791.76	kJ/mol	Joback Method
hfus	57.53	kJ/mol	Joback Method
hvap	89.61	kJ/mol	Joback Method
log10ws	-6.70		Crippen Method
logp	6.017		Crippen Method
mcvol	340.140	ml/mol	McGowan Method
pc	1041.25	kPa	Joback Method
rinsol	2983.00		NIST Webbook
tb	927.78	K	Joback Method
tc	1136.42	K	Joback Method
tf	530.98	K	Joback Method
vc	1.319	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1119.96	J/molxK	927.78	Joback Method
cpg	1137.09	J/molxK	962.55	Joback Method
cpg	1152.87	J/molxK	997.33	Joback Method
cpg	1167.34	J/molxK	1032.10	Joback Method
cpg	1180.56	J/molxK	1066.87	Joback Method
cpg	1192.57	J/molxK	1101.65	Joback Method
cpg	1203.40	J/molxK	1136.42	Joback Method
dvisc	0.0004449	Paxs	530.98	Joback Method
dvisc	0.0002217	Paxs	597.11	Joback Method

dvisc	0.0001269	Paxs	663.25	Joback Method
dvisc	0.0000804	Paxs	729.38	Joback Method
dvisc	0.0000549	Paxs	795.51	Joback Method
dvisc	0.0000398	Paxs	861.65	Joback Method
dvisc	0.0000302	Paxs	927.78	Joback Method

Sources

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=U354388&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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