

Sebacic acid, pentyl 1-phenylpropyl ester

Inchi: InChI=1S/C24H38O4/c1-3-5-15-20-27-23(25)18-13-8-6-7-9-14-19-24(26)28-22(4-2)21-16
InchiKey: MQVUXRXWGRUIFY-UHFFFAOYSA-N
Formula: C24H38O4
SMILES: CCCCCOC(=O)CCCCCCCCC(=O)OC(CC)c1ccccc1
Mol. weight [g/mol]: 390.56

Physical Properties

Property code	Value	Unit	Source
gf	-206.67	kJ/mol	Joback Method
hf	-797.04	kJ/mol	Joback Method
hfus	54.01	kJ/mol	Joback Method
hvap	89.22	kJ/mol	Joback Method
log10ws	-7.16		Crippen Method
logp	6.535		Crippen Method
mcvol	340.140	ml/mol	McGowan Method
pc	1046.65	kPa	Joback Method
rinpol	2769.00		NIST Webbook
tb	927.34	K	Joback Method
tc	1136.36	K	Joback Method
tf	515.98	K	Joback Method
vc	1.313	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1120.39	J/mol×K	927.34	Joback Method
cpg	1192.82	J/mol×K	1101.52	Joback Method
cpg	1180.88	J/mol×K	1066.69	Joback Method
cpg	1167.71	J/mol×K	1031.85	Joback Method
cpg	1153.27	J/mol×K	997.01	Joback Method
cpg	1137.51	J/mol×K	962.18	Joback Method
cpg	1203.56	J/mol×K	1136.36	Joback Method
dvisc	0.0000275	Pa×s	927.34	Joback Method
dvisc	0.0000368	Pa×s	858.78	Joback Method

dvisc	0.0000518	Pa×s	790.22	Joback Method
dvisc	0.0000778	Pa×s	721.66	Joback Method
dvisc	0.0001272	Pa×s	653.10	Joback Method
dvisc	0.0002333	Pa×s	584.54	Joback Method
dvisc	0.0005027	Pa×s	515.98	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U354988&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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