

Sebacic acid, hexyl 3-phenylallyl ester

Inchi:	InChI=1S/C25H38O4/c1-2-3-4-14-21-28-24(26)19-12-7-5-6-8-13-20-25(27)29-22-15-18-2
InchiKey:	UUVQWXDKHIMDEH-OBGWFSINSA-N
Formula:	C25H38O4
SMILES:	CCCCCOC(=O)CCCCCCCC(=O)OCC=Cc1ccccc1
Mol. weight [g/mol]:	402.57

Physical Properties

Property code	Value	Unit	Source
gf	-115.59	kJ/mol	Joback Method
hf	-695.18	kJ/mol	Joback Method
hfus	60.32	kJ/mol	Joback Method
hvap	91.79	kJ/mol	Joback Method
log10ws	-7.14		Crippen Method
logp	6.487		Crippen Method
mvol	349.930	ml/mol	McGowan Method
pc	1012.30	kPa	Joback Method
rinpol	3110.00		NIST Webbook
rinpol	3110.00		NIST Webbook
tb	954.82	K	Joback Method
tc	1169.21	K	Joback Method
tf	537.17	K	Joback Method
vc	1.355	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1153.74	J/molxK	954.82	Joback Method
cpg	1226.59	J/molxK	1133.48	Joback Method
cpg	1214.34	J/molxK	1097.75	Joback Method
cpg	1200.99	J/molxK	1062.02	Joback Method
cpg	1186.48	J/molxK	1026.28	Joback Method
cpg	1170.75	J/molxK	990.55	Joback Method
cpg	1237.81	J/molxK	1169.21	Joback Method
dvisc	0.0000227	Paxs	954.82	Joback Method

dvisc	0.0000301	Paxs	885.21	Joback Method
dvisc	0.0000419	Paxs	815.60	Joback Method
dvisc	0.0000618	Paxs	745.99	Joback Method
dvisc	0.0000990	Paxs	676.39	Joback Method
dvisc	0.0001765	Paxs	606.78	Joback Method
dvisc	0.0003657	Paxs	537.17	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=U355892&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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