

Sebacic acid, heptyl 3-phenylallyl ester

Inchi:	InChI=1S/C26H40O4/c1-2-3-4-9-15-22-29-25(27)20-13-7-5-6-8-14-21-26(28)30-23-16-19
InchiKey:	SZZFTEMAEOTPFR-KNTRCKAVSA-N
Formula:	C26H40O4
SMILES:	CCCCCCCOC(=O)CCCCCCCC(=O)OCC=Cc1ccccc1
Mol. weight [g/mol]:	416.59

Physical Properties

Property code	Value	Unit	Source
gf	-107.17	kJ/mol	Joback Method
hf	-715.82	kJ/mol	Joback Method
hfus	62.91	kJ/mol	Joback Method
hvap	94.02	kJ/mol	Joback Method
log10ws	-7.55		Crippen Method
logp	6.877		Crippen Method
mvol	364.020	ml/mol	McGowan Method
pc	953.19	kPa	Joback Method
rinpol	3209.00		NIST Webbook
rinpol	3209.00		NIST Webbook
tb	977.70	K	Joback Method
tc	1197.03	K	Joback Method
tf	548.44	K	Joback Method
vc	1.411	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1215.88	J/molxK	977.70	Joback Method
cpg	1233.23	J/molxK	1014.25	Joback Method
cpg	1249.22	J/molxK	1050.81	Joback Method
cpg	1263.94	J/molxK	1087.36	Joback Method
cpg	1277.45	J/molxK	1123.92	Joback Method
cpg	1289.83	J/molxK	1160.47	Joback Method
cpg	1301.14	J/molxK	1197.03	Joback Method
dvisc	0.0003232	Paxs	548.44	Joback Method

dvisc	0.0001546	Paxs	619.98	Joback Method
dvisc	0.0000861	Paxs	691.53	Joback Method
dvisc	0.0000536	Paxs	763.07	Joback Method
dvisc	0.0000361	Paxs	834.61	Joback Method
dvisc	0.0000259	Paxs	906.16	Joback Method
dvisc	0.0000195	Paxs	977.70	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=U355893&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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