

Sebacic acid, decyl phenyl ester

Inchi:	InChI=1S/C26H42O4/c1-2-3-4-5-6-9-12-18-23-29-25(27)21-16-10-7-8-11-17-22-26(28)30
InchiKey:	IBDGXRVAECCOFA-UHFFFAOYSA-N
Formula:	C26H42O4
SMILES:	CCCCCCCCCOC(=O)CCCCCCCC(=O)Oc1ccccc1
Mol. weight [g/mol]:	418.61

Physical Properties

Property code	Value	Unit	Source
gf	-187.39	kJ/mol	Joback Method
hf	-833.04	kJ/mol	Joback Method
hfus	62.71	kJ/mol	Joback Method
hvap	94.06	kJ/mol	Joback Method
log10ws	-8.18		Crippen Method
logp	7.397		Crippen Method
mvol	368.320	ml/mol	McGowan Method
pc	923.30	kPa	Joback Method
rinpol	3189.00		NIST Webbook
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tb	973.54	K	Joback Method
tc	1192.35	K	Joback Method
tf	553.52	K	Joback Method
vc	1.431	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1244.21	J/molxK	973.54	Joback Method
cpg	1318.16	J/molxK	1155.88	Joback Method
cpg	1306.17	J/molxK	1119.41	Joback Method
cpg	1292.83	J/molxK	1082.94	Joback Method
cpg	1278.10	J/molxK	1046.48	Joback Method
cpg	1261.91	J/molxK	1010.01	Joback Method
cpg	1328.87	J/molxK	1192.35	Joback Method
dvisc	0.0000223	Paxs	973.54	Joback Method

dvisc	0.0000295	Paxs	903.54	Joback Method
dvisc	0.0000409	Paxs	833.53	Joback Method
dvisc	0.0000603	Paxs	763.53	Joback Method
dvisc	0.0000962	Paxs	693.53	Joback Method
dvisc	0.0001703	Paxs	623.52	Joback Method
dvisc	0.0003484	Paxs	553.52	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=U354514&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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