

Phthalic acid, 2,5-dichlorobenzyl decyl ester

Inchi:	InChI=1S/C25H30Cl2O4/c1-2-3-4-5-6-7-8-11-16-30-24(28)21-12-9-10-13-22(21)25(29)3
InchiKey:	VJHLIFIENCKONI-UHFFFAOYSA-N
Formula:	C25H30Cl2O4
SMILES:	CCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cc(Cl)ccc1Cl
Mol. weight [g/mol]:	465.41

Physical Properties

Property code	Value	Unit	Source
gf	-136.15	kJ/mol	Joback Method
hf	-641.76	kJ/mol	Joback Method
hfus	61.39	kJ/mol	Joback Method
hvap	104.86	kJ/mol	Joback Method
log10ws	-9.20		Crippen Method
logp	7.648		Crippen Method
mvol	354.950	ml/mol	McGowan Method
pc	1123.81	kPa	Joback Method
rinpol	3220.00		NIST Webbook
rinpol	3220.00		NIST Webbook
tb	1067.14	K	Joback Method
tc	1307.11	K	Joback Method
tf	666.07	K	Joback Method
vc	1.365	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1117.37	J/molxK	1067.14	Joback Method
cpg	1128.87	J/molxK	1107.14	Joback Method
cpg	1138.87	J/molxK	1147.13	Joback Method
cpg	1147.42	J/molxK	1187.13	Joback Method
cpg	1154.58	J/molxK	1227.12	Joback Method
cpg	1160.41	J/molxK	1267.12	Joback Method
cpg	1164.96	J/molxK	1307.11	Joback Method
dvisc	0.0001613	Paxs	666.07	Joback Method

dvisc	0.0000978	Paxs	732.92	Joback Method
dvisc	0.0000644	Paxs	799.76	Joback Method
dvisc	0.0000453	Paxs	866.61	Joback Method
dvisc	0.0000335	Paxs	933.45	Joback Method
dvisc	0.0000258	Paxs	1000.30	Joback Method
dvisc	0.0000205	Paxs	1067.14	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=U382919&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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