

Phthalic acid, decyl 2,4,6-trichlorobenzyl ester

Inchi: InChI=1S/C25H29Cl3O4/c1-2-3-4-5-6-7-8-11-14-31-24(29)19-12-9-10-13-20(19)25(30)31
InchiKey: ISCOTEXXDLPMAR-UHFFFAOYSA-N
Formula: C25H29Cl3O4
SMILES: CCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]: 499.85

Physical Properties

Property code	Value	Unit	Source
gf	-157.71	kJ/mol	Joback Method
hf	-668.97	kJ/mol	Joback Method
hfus	65.20	kJ/mol	Joback Method
hvap	109.91	kJ/mol	Joback Method
log10ws	-9.89		Crippen Method
logp	8.301		Crippen Method
mvol	367.190	ml/mol	McGowan Method
pc	1085.63	kPa	Joback Method
rinpol	3358.00		NIST Webbook
rinpol	3358.00		NIST Webbook
tb	1109.55	K	Joback Method
tc	1358.42	K	Joback Method
tf	708.51	K	Joback Method
vc	1.415	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1133.94	J/molxK	1109.55	Joback Method
cpg	1143.84	J/molxK	1151.03	Joback Method
cpg	1152.17	J/molxK	1192.51	Joback Method
cpg	1158.97	J/molxK	1233.98	Joback Method
cpg	1164.32	J/molxK	1275.46	Joback Method
cpg	1168.26	J/molxK	1316.94	Joback Method
cpg	1170.85	J/molxK	1358.42	Joback Method
dvisc	0.0001210	Paxs	708.51	Joback Method

dvisc	0.0000764	Paxs	775.35	Joback Method
dvisc	0.0000519	Paxs	842.19	Joback Method
dvisc	0.0000373	Paxs	909.03	Joback Method
dvisc	0.0000281	Paxs	975.87	Joback Method
dvisc	0.0000219	Paxs	1042.71	Joback Method
dvisc	0.0000176	Paxs	1109.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382884&Units=SI
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

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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