Phthalic acid, 2,5-dichlorobenzyl undecyl ester

Inchi: InChI=1S/C26H32Cl2O4/c1-2-3-4-5-6-7-8-9-12-17-31-25(29)22-13-10-11-14-23(22)26(30
InchiKey: MZHQUPHSFHTVPI-UHFFFAOYSA-N
Formula: C26H32Cl2O4
SMILES: CCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cc(Cl)ccc1Cl
Mol. weight [g/mol]: 479.44

Physical Properties

Property code	Value	Unit	Source
gf	-127.73	kJ/mol	Joback Method
hf	-662.40	kJ/mol	Joback Method
hfus	63.98	kJ/mol	Joback Method
hvap	107.09	kJ/mol	Joback Method
log10ws	-9.62		Crippen Method
logp	8.038		Crippen Method
mcvol	369.040	ml/mol	McGowan Method
pc	1054.83	kPa	Joback Method
rinpol	3322.00		NIST Webbook
rinpol	3322.00		NIST Webbook
tb	1090.02	K	Joback Method
tc	1334.49	K	Joback Method
tf	677.34	K	Joback Method
vc	1.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1177.56	J/mol×K	1090.02	Joback Method
cpg	1220.29	J/mol×K	1293.75	Joback Method
cpg	1214.63	J/mol×K	1253.00	Joback Method
cpg	1207.59	J/mol×K	1212.26	Joback Method
cpg	1199.11	J/mol×K	1171.51	Joback Method
cpg	1189.12	J/mol×K	1130.77	Joback Method
cpg	1224.65	J/mol×K	1334.49	Joback Method
dvisc	0.0000176	Pa×s	1090.02	Joback Method

dvisc	0.0000221	Pa×s	1021.24	Joback Method
dvisc	0.0000289	Pa×s	952.46	Joback Method
dvisc	0.0000392	Pa×s	883.68	Joback Method
dvisc	0.0000561	Pa×s	814.90	Joback Method
dvisc	0.0000857	Pa×s	746.12	Joback Method
dvisc	0.0001428	Pa×s	677.34	Joback Method

Sources

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=U382920&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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