

Phthalic acid, 2,4-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)27-28
InchiKey: XCVOXVMTUBHQTR-UHFFFAOYSA-N
Formula: C26H32Cl2O4
SMILES: CCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccc(Cl)cc1Cl
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
mvol	369.040	ml/mol	McGowan Method
pc	1054.83	kPa	Joback Method
rinpol	3295.00		NIST Webbook
rinpol	3295.00		NIST Webbook
tb	1090.02	K	Joback Method
tc	1334.49	K	Joback Method
tf	677.34	K	Joback Method
vc	1.421	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0000221	Paxs	1021.24	Joback Method
dvisc	0.0000289	Paxs	952.46	Joback Method
dvisc	0.0000392	Paxs	883.68	Joback Method
dvisc	0.0000561	Paxs	814.90	Joback Method
dvisc	0.0000857	Paxs	746.12	Joback Method
dvisc	0.0001428	Paxs	677.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382567&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
mccvol:	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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