

Phthalic acid, 4-chloro-2-methoxybenzyl octyl ester

Inchi:	InChI=1S/C24H29ClO5/c1-3-4-5-6-7-10-15-29-23(26)20-11-8-9-12-21(20)24(27)30-17-18
InchiKey:	KMBAUBTYCMIFGQ-UHFFFAOYSA-N
Formula:	C24H29ClO5
SMILES:	CCCCCCCCOC(=O)c1cccc1C(=O)OCc1ccc(Cl)cc1OC
Mol. weight [g/mol]:	432.94

Physical Properties

Property code	Value	Unit	Source
gf	-237.64	kJ/mol	Joback Method
hf	-737.60	kJ/mol	Joback Method
hfus	55.79	kJ/mol	Joback Method
hvap	100.66	kJ/mol	Joback Method
log10ws	-7.80		Crippen Method
logp	6.223		Crippen Method
mvol	334.490	ml/mol	McGowan Method
pc	1216.59	kPa	Joback Method
rinpol	3071.00		NIST Webbook
rinpol	3071.00		NIST Webbook
tb	1029.25	K	Joback Method
tc	1262.24	K	Joback Method
tf	647.11	K	Joback Method
vc	1.278	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1063.03	J/molxK	1029.25	Joback Method
cpg	1074.69	J/molxK	1068.08	Joback Method
cpg	1084.70	J/molxK	1106.91	Joback Method
cpg	1093.09	J/molxK	1145.75	Joback Method
cpg	1099.89	J/molxK	1184.58	Joback Method
cpg	1105.13	J/molxK	1223.41	Joback Method
cpg	1108.83	J/molxK	1262.24	Joback Method
dvisc	0.0001572	Paxs	647.11	Joback Method

dvisc	0.0000966	Paxs	710.80	Joback Method
dvisc	0.0000644	Paxs	774.49	Joback Method
dvisc	0.0000456	Paxs	838.18	Joback Method
dvisc	0.0000339	Paxs	901.87	Joback Method
dvisc	0.0000262	Paxs	965.56	Joback Method
dvisc	0.0000209	Paxs	1029.25	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=U382842&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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