Phthalic acid, 2-(4-chlorophenyl)ethyl pentyl ester

Inchi: InChI=1S/C21H23ClO4/c1-2-3-6-14-25-20(23)18-7-4-5-8-19(18)21(24)26-15-13-16-9-11-

InchiKey: YPDWJAREUJJKDQ-UHFFFAOYSA-N

Formula: C21H23ClO4

SMILES: CCCCCOC(=O)c1ccccc1C(=O)OCCc1ccc(Cl)cc1

Mol. weight [g/mol]: 374.86

Physical Properties

Property code	Value	Unit	Source
gf	-148.27	kJ/mol	Joback Method
hf	-531.99	kJ/mol	Joback Method
hfus	47.22	kJ/mol	Joback Method
hvap	90.91	kJ/mol	Joback Method
log10ws	-6.35		Crippen Method
logp	5.086		Crippen Method
mcvol	286.350	ml/mol	McGowan Method
pc	1541.49	kPa	Joback Method
rinpol	2798.00		NIST Webbook
rinpol	2798.00		NIST Webbook
tb	933.21	K	Joback Method
tc	1160.36	K	Joback Method
tf	578.55	K	Joback Method
vc	1.093	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	861.25	J/mol×K	933.21	Joback Method
cpg	912.52	J/mol×K	1122.50	Joback Method
cpg	904.71	J/mol×K	1084.65	Joback Method
cpg	895.72	J/mol×K	1046.79	Joback Method
cpg	885.51	J/mol×K	1008.93	Joback Method
cpg	874.03	J/mol×K	971.07	Joback Method
cpg	919.18	J/mol×K	1160.36	Joback Method
dvisc	0.0000429	Pa×s	933.21	Joback Method

dvisc	0.0000540	Pa×s	874.10	Joback Method
dvisc	0.0000701	Pa×s	814.99	Joback Method
dvisc	0.0000950	Pa×s	755.88	Joback Method
dvisc	0.0001354	Pa×s	696.77	Joback Method
dvisc	0.0002062	Pa×s	637.66	Joback Method
dvisc	0.0003421	Pa×s	578.55	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=U377839&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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