Isophthalic acid, 2,4-dichlorophenyl heptyl ester

Inchi: InChI=1S/C21H22Cl2O4/c1-2-3-4-5-6-12-26-20(24)15-8-7-9-16(13-15)21(25)27-19-11-10

InchiKey: BMGJUHHOVHKCTE-UHFFFAOYSA-N

Formula: C21H22Cl2O4

SMILES: CCCCCCCOC(=O)c1cccc(C(=O)Oc2ccc(Cl)cc2Cl)c1

Mol. weight [g/mol]: 409.30

Physical Properties

Property code	Value	Unit	Source
gf	-169.83	kJ/mol	Joback Method
hf	-559.20	kJ/mol	Joback Method
hfus	51.03	kJ/mol	Joback Method
hvap	95.96	kJ/mol	Joback Method
log10ws	-7.68		Crippen Method
logp	6.340		Crippen Method
mcvol	298.590	ml/mol	McGowan Method
pc	1480.43	kPa	Joback Method
rinpol	3131.00		NIST Webbook
rinpol	3131.00		NIST Webbook
tb	975.62	K	Joback Method
tc	1207.92	K	Joback Method
tf	620.99	K	Joback Method
vc	1.141	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	880.88	J/mol×K	975.62	Joback Method
cpg	892.17	J/mol×K	1014.34	Joback Method
cpg	902.14	J/mol×K	1053.05	Joback Method
cpg	910.83	J/mol×K	1091.77	Joback Method
cpg	918.26	J/mol×K	1130.49	Joback Method
cpg	924.49	J/mol×K	1169.20	Joback Method
cpg	929.54	J/mol×K	1207.92	Joback Method
dvisc	0.0002554	Pa×s	620.99	Joback Method

dvisc	0.0001614	Pa×s	680.10	Joback Method
dvisc	0.0001098	Pa×s	739.20	Joback Method
dvisc	0.0000790	Pa×s	798.30	Joback Method
dvisc	0.0000595	Pa×s	857.41	Joback Method
dvisc	0.0000465	Pa×s	916.51	Joback Method
dvisc	0.0000375	Pa×s	975.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344411&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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