Isophthalic acid, hexyl 2,3,5-trichlorophenyl ester

Inchi: InChI=1S/C20H19Cl3O4/c1-2-3-4-5-9-26-19(24)13-7-6-8-14(10-13)20(25)27-17-12-15(21

InchiKey: RPLPAPLQJHADGI-UHFFFAOYSA-N

Formula: C20H19Cl3O4

SMILES: CCCCCCOC(=O)c1cccc(C(=O)Oc2cc(Cl)cc(Cl)c2Cl)c1

Mol. weight [g/mol]: 429.72

Physical Properties

Property code	Value	Unit	Source
gf	-199.81	kJ/mol	Joback Method
hf	-565.77	kJ/mol	Joback Method
hfus	52.25	kJ/mol	Joback Method
hvap	98.78	kJ/mol	Joback Method
log10ws	-7.95		Crippen Method
logp	6.603		Crippen Method
mcvol	296.740	ml/mol	McGowan Method
pc	1531.86	kPa	Joback Method
rinpol	3083.00		NIST Webbook
rinpol	3083.00		NIST Webbook
tb	995.15	K	Joback Method
tc	1232.78	K	Joback Method
tf	652.16	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	840.52	J/mol×K	995.15	Joback Method
cpg	850.24	J/mol×K	1034.75	Joback Method
cpg	858.64	J/mol×K	1074.36	Joback Method
cpg	865.76	J/mol×K	1113.96	Joback Method
cpg	871.62	J/mol×K	1153.57	Joback Method
cpg	876.24	J/mol×K	1193.17	Joback Method
cpg	879.67	J/mol×K	1232.78	Joback Method
dvisc	0.0002166	Pa×s	652.16	Joback Method

dvisc	0.0001439	Pa×s	709.32	Joback Method
dvisc	0.0001017	Pa×s	766.49	Joback Method
dvisc	0.0000754	Pa×s	823.65	Joback Method
dvisc	0.0000581	Pa×s	880.82	Joback Method
dvisc	0.0000462	Pa×s	937.98	Joback Method
dvisc	0.0000377	Pa×s	995.15	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356622&Units=SI

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