1,2-Cyclohexanedicarboxylic acid, hexyl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C20H25Cl3O4/c1-2-3-4-7-10-26-19(24)14-8-5-6-9-15(14)20(25)27-18-16(22)11

InchiKey: MUVXKQDJIMUPLM-UHFFFAOYSA-N

Formula: C20H25Cl3O4

SMILES: CCCCCCOC(=O)C1CCCCC1C(=O)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 435.77

Physical Properties

Property code	Value	Unit	Source
gf	-285.85	kJ/mol	Joback Method
hf	-756.85	kJ/mol	Joback Method
hfus	51.50	kJ/mol	Joback Method
hvap	95.96	kJ/mol	Joback Method
log10ws	-7.14		Crippen Method
logp	6.482		Crippen Method
mcvol	309.640	ml/mol	McGowan Method
pc	1372.76	kPa	Joback Method
rinpol	2868.00		NIST Webbook
rinpol	2868.00		NIST Webbook
tb	978.37	K	Joback Method
tc	1211.12	K	Joback Method
tf	616.36	K	Joback Method
vc	1.175	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	948.09	J/mol×K	978.37	Joback Method
cpg	992.85	J/mol×K	1172.33	Joback Method
cpg	987.09	J/mol×K	1133.54	Joback Method
cpg	979.75	J/mol×K	1094.75	Joback Method
cpg	970.82	J/mol×K	1055.95	Joback Method
cpg	960.27	J/mol×K	1017.16	Joback Method
cpg	997.06	J/mol×K	1211.12	Joback Method
dvisc	0.0000488	Pa×s	978.37	Joback Method

dvisc	0.0000605	Pa×s	918.04	Joback Method
dvisc	0.0000773	Pa×s	857.70	Joback Method
dvisc	0.0001025	Pa×s	797.37	Joback Method
dvisc	0.0001424	Pa×s	737.03	Joback Method
dvisc	0.0002098	Pa×s	676.70	Joback Method
dvisc	0.0003333	Pa×s	616.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339811&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
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
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