

1,2-Cyclohexanedicarboxylic acid, butyl 2,5-dichlorophenyl ester

Inchi:	InChI=1S/C18H22Cl2O4/c1-2-3-10-23-17(21)13-6-4-5-7-14(13)18(22)24-16-11-12(19)8-9
InchiKey:	OLZMJJFEDMHOJM-UHFFFAOYSA-N
Formula:	C18H22Cl2O4
SMILES:	CCCCOC(=O)C1CCCCC1C(=O)Oc1cc(Cl)ccc1Cl
Mol. weight [g/mol]:	373.27

Physical Properties

Property code	Value	Unit	Source
gf	-281.13	kJ/mol	Joback Method
hf	-688.36	kJ/mol	Joback Method
hfus	42.51	kJ/mol	Joback Method
hvap	86.46	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	5.048		Crippen Method
mvol	269.220	ml/mol	McGowan Method
pc	1659.19	kPa	Joback Method
rinpol	2532.00		NIST Webbook
rinpol	2532.00		NIST Webbook
tb	890.20	K	Joback Method
tc	1120.39	K	Joback Method
tf	551.38	K	Joback Method
vc	1.014	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	810.29	J/molxK	890.20	Joback Method
cpg	824.42	J/molxK	928.56	Joback Method
cpg	837.02	J/molxK	966.93	Joback Method
cpg	848.11	J/molxK	1005.29	Joback Method
cpg	857.71	J/molxK	1043.66	Joback Method
cpg	865.83	J/molxK	1082.02	Joback Method
cpg	872.49	J/molxK	1120.39	Joback Method
dvisc	0.0005472	Paxs	551.38	Joback Method

dvisc	0.0003362	Paxs	607.85	Joback Method
dvisc	0.0002243	Paxs	664.32	Joback Method
dvisc	0.0001595	Paxs	720.79	Joback Method
dvisc	0.0001192	Paxs	777.26	Joback Method
dvisc	0.0000926	Paxs	833.73	Joback Method
dvisc	0.0000743	Paxs	890.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339798&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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