

1,2-Cyclohexanedicarboxylic acid, butyl isopropyl ester

Inchi:	InChI=1S/C15H26O4/c1-4-5-10-18-14(16)12-8-6-7-9-13(12)15(17)19-11(2)3/h11-13H,4-
InchiKey:	FWQZJWWALZJRLI-UHFFFAOYSA-N
Formula:	C15H26O4
SMILES:	CCCCOC(=O)C1CCCCC1C(=O)OC(C)C
Mol. weight [g/mol]:	270.36

Physical Properties

Property code	Value	Unit	Source
gf	-378.12	kJ/mol	Joback Method
hf	-813.83	kJ/mol	Joback Method
hfus	29.56	kJ/mol	Joback Method
hvap	67.03	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	3.088		Crippen Method
mvol	226.230	ml/mol	McGowan Method
pc	1756.54	kPa	Joback Method
rinpol	1952.00		NIST Webbook
tb	709.62	K	Joback Method
tc	910.33	K	Joback Method
tf	391.27	K	Joback Method
vc	0.850	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	674.70	J/molxK	709.62	Joback Method
cpg	693.58	J/molxK	743.07	Joback Method
cpg	711.32	J/molxK	776.52	Joback Method
cpg	727.90	J/molxK	809.98	Joback Method
cpg	743.34	J/molxK	843.43	Joback Method
cpg	757.63	J/molxK	876.88	Joback Method
cpg	770.79	J/molxK	910.33	Joback Method
dvisc	0.0019030	Paxs	391.27	Joback Method
dvisc	0.0009222	Paxs	444.33	Joback Method

dvisc	0.0005216	Paxs	497.39	Joback Method
dvisc	0.0003292	Paxs	550.44	Joback Method
dvisc	0.0002254	Paxs	603.50	Joback Method
dvisc	0.0001640	Paxs	656.56	Joback Method
dvisc	0.0001251	Paxs	709.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339637&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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