

1,2-Cyclohexanedicarboxylic acid, butyl 2-cyclohexylethyl ester

Inchi:	InChI=1S/C20H34O4/c1-2-3-14-23-19(21)17-11-7-8-12-18(17)20(22)24-15-13-16-9-5-4-6
InchiKey:	FSAPWUZNEKMZSJ-UHFFFAOYSA-N
Formula:	C20H34O4
SMILES:	CCCCOC(=O)C1CCCCC1C(=O)OCCC1CCCCC1
Mol. weight [g/mol]:	338.48

Physical Properties

Property code	Value	Unit	Source
gf	-309.13	kJ/mol	Joback Method
hf	-857.43	kJ/mol	Joback Method
hfus	37.87	kJ/mol	Joback Method
hvap	78.97	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.650		Crippen Method
mvol	285.820	ml/mol	McGowan Method
pc	1403.79	kPa	Joback Method
rinpol	2402.00		NIST Webbook
rinpol	2402.00		NIST Webbook
tb	844.01	K	Joback Method
tc	1057.86	K	Joback Method
tf	470.00	K	Joback Method
vc	1.069	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	966.74	J/molxK	844.01	Joback Method
cpg	987.02	J/molxK	879.65	Joback Method
cpg	1005.59	J/molxK	915.29	Joback Method
cpg	1022.47	J/molxK	950.94	Joback Method
cpg	1037.69	J/molxK	986.58	Joback Method
cpg	1051.27	J/molxK	1022.22	Joback Method
cpg	1063.24	J/molxK	1057.86	Joback Method
dvisc	0.0011636	Paxs	470.00	Joback Method

dvisc	0.0005606	Paxs	532.34	Joback Method
dvisc	0.0003148	Paxs	594.67	Joback Method
dvisc	0.0001972	Paxs	657.00	Joback Method
dvisc	0.0001340	Paxs	719.34	Joback Method
dvisc	0.0000968	Paxs	781.67	Joback Method
dvisc	0.0000734	Paxs	844.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339725&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

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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