

1,2-Cyclohexanedicarboxylic acid, butyl cyclohexylmethyl ester

Inchi:	InChI=1S/C19H32O4/c1-2-3-13-22-18(20)16-11-7-8-12-17(16)19(21)23-14-15-9-5-4-6-10
InchiKey:	JPHBWSLDRQHZFP-UHFFFAOYSA-N
Formula:	C19H32O4
SMILES:	CCCCOC(=O)C1CCCCC1C(=O)OCC1CCCCC1
Mol. weight [g/mol]:	324.45

Physical Properties

Property code	Value	Unit	Source
gf	-317.55	kJ/mol	Joback Method
hf	-836.79	kJ/mol	Joback Method
hfus	35.28	kJ/mol	Joback Method
hvap	76.75	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	4.260		Crippen Method
mvol	271.730	ml/mol	McGowan Method
pc	1510.50	kPa	Joback Method
rinpol	2304.00		NIST Webbook
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tb	821.13	K	Joback Method
tc	1036.41	K	Joback Method
tf	458.73	K	Joback Method
vc	1.012	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	905.80	J/molxK	821.13	Joback Method
cpg	926.29	J/molxK	857.01	Joback Method
cpg	945.10	J/molxK	892.89	Joback Method
cpg	962.23	J/molxK	928.77	Joback Method
cpg	977.73	J/molxK	964.65	Joback Method
cpg	991.60	J/molxK	1000.53	Joback Method
cpg	1003.86	J/molxK	1036.41	Joback Method
dvisc	0.0012919	Paxs	458.73	Joback Method

dvisc	0.0006292	Paxs	519.13	Joback Method
dvisc	0.0003560	Paxs	579.53	Joback Method
dvisc	0.0002243	Paxs	639.93	Joback Method
dvisc	0.0001530	Paxs	700.33	Joback Method
dvisc	0.0001109	Paxs	760.73	Joback Method
dvisc	0.0000843	Paxs	821.13	Joback Method

Sources

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=U339739&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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