

1,2-Cyclohexanedicarboxylic acid, butyl cyclohex-3-enylmethyl ester

Inchi:	InChI=1S/C19H30O4/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:	WWVDZEGDUSTVJQ-UHFFFAOYSA-N
Formula:	C19H30O4
SMILES:	CCCCOC(=O)C1CCCCC1C(=O)OCC1CC=CCC1
Mol. weight [g/mol]:	322.44

Physical Properties

Property code	Value	Unit	Source
gf	-287.59	kJ/mol	Joback Method
hf	-779.01	kJ/mol	Joback Method
hfus	36.50	kJ/mol	Joback Method
hvap	77.04	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	4.036		Crippen Method
mcvol	267.430	ml/mol	McGowan Method
pc	1553.67	kPa	Joback Method
rinqol	2320.00		NIST Webbook
tb	820.29	K	Joback Method
tc	1036.84	K	Joback Method
tf	459.49	K	Joback Method
vc	0.999	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	878.02	J/molxK	820.29	Joback Method
cpg	897.74	J/molxK	856.38	Joback Method
cpg	915.81	J/molxK	892.47	Joback Method
cpg	932.25	J/molxK	928.57	Joback Method
cpg	947.10	J/molxK	964.66	Joback Method
cpg	960.36	J/molxK	1000.75	Joback Method
cpg	972.08	J/molxK	1036.84	Joback Method
dvisc	0.0012502	Paxs	459.49	Joback Method
dvisc	0.0006268	Paxs	519.62	Joback Method

dvisc	0.0003627	Paxs	579.76	Joback Method
dvisc	0.0002326	Paxs	639.89	Joback Method
dvisc	0.0001610	Paxs	700.02	Joback Method
dvisc	0.0001181	Paxs	760.16	Joback Method
dvisc	0.0000907	Paxs	820.29	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339868&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mccvol:	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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