

1,2-Cyclohexanedicarboxylic acid, butyl heptyl ester

Inchi:	InChI=1S/C19H34O4/c1-3-5-7-8-11-15-23-19(21)17-13-10-9-12-16(17)18(20)22-14-6-4-2
InchiKey:	SCPRZDYCGCTIMW-UHFFFAOYSA-N
Formula:	C19H34O4
SMILES:	CCCCCCCOC(=O)C1CCCCC1C(=O)OCCCC
Mol. weight [g/mol]:	326.47

Physical Properties

Property code	Value	Unit	Source
gf	-342.00	kJ/mol	Joback Method
hf	-891.11	kJ/mol	Joback Method
hfus	43.45	kJ/mol	Joback Method
hvap	76.32	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	4.650		Crippen Method
mcvol	282.590	ml/mol	McGowan Method
pc	1295.79	kPa	Joback Method
rinpol	2216.00		NIST Webbook
rinpol	2216.00		NIST Webbook
tb	801.58	K	Joback Method
tc	996.17	K	Joback Method
tf	451.35	K	Joback Method
vc	1.079	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.76	J/molxK	801.58	Joback Method
cpg	991.95	J/molxK	963.74	Joback Method
cpg	977.79	J/molxK	931.31	Joback Method
cpg	962.41	J/molxK	898.87	Joback Method
cpg	945.79	J/molxK	866.44	Joback Method
cpg	927.91	J/molxK	834.01	Joback Method
cpg	1004.88	J/molxK	996.17	Joback Method
dvisc	0.0000810	Paxs	801.58	Joback Method

dvisc	0.0001057	Paxs	743.21	Joback Method
dvisc	0.0001443	Paxs	684.84	Joback Method
dvisc	0.0002087	Paxs	626.46	Joback Method
dvisc	0.0003257	Paxs	568.09	Joback Method
dvisc	0.0005626	Paxs	509.72	Joback Method
dvisc	0.0011198	Paxs	451.35	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339534&Units=SI

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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