

1,2-Cyclohexanedicarboxylic acid, isobutyl octyl ester

Inchi:	InChI=1S/C20H36O4/c1-4-5-6-7-8-11-14-23-19(21)17-12-9-10-13-18(17)20(22)24-15-16
InchiKey:	KXQYQKVACIQHEL-UHFFFAOYSA-N
Formula:	C20H36O4
SMILES:	CCCCCCCCOC(=O)C1CCCCC1C(=O)OCC(C)C
Mol. weight [g/mol]:	340.50

Physical Properties

Property code	Value	Unit	Source
gf	-336.02	kJ/mol	Joback Method
hf	-917.03	kJ/mol	Joback Method
hfus	42.51	kJ/mol	Joback Method
hvap	78.16	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.896		Crippen Method
mvol	296.680	ml/mol	McGowan Method
pc	1217.44	kPa	Joback Method
rinpol	2279.00		NIST Webbook
rinpol	2279.00		NIST Webbook
tb	824.02	K	Joback Method
tc	1020.98	K	Joback Method
tf	447.62	K	Joback Method
vc	1.129	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.98	J/molxK	824.02	Joback Method
cpg	989.40	J/molxK	856.85	Joback Method
cpg	1007.46	J/molxK	889.67	Joback Method
cpg	1024.18	J/molxK	922.50	Joback Method
cpg	1039.58	J/molxK	955.33	Joback Method
cpg	1053.69	J/molxK	988.16	Joback Method
cpg	1066.50	J/molxK	1020.98	Joback Method
dvisc	0.0011819	Paxs	447.62	Joback Method

dvisc	0.0005412	Paxs	510.35	Joback Method
dvisc	0.0002940	Paxs	573.09	Joback Method
dvisc	0.0001802	Paxs	635.82	Joback Method
dvisc	0.0001206	Paxs	698.55	Joback Method
dvisc	0.0000862	Paxs	761.29	Joback Method
dvisc	0.0000648	Paxs	824.02	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=U339429&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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