

1,2-Cyclohexanedicarboxylic acid, isobutyl nonyl ester

Inchi:	InChI=1S/C21H38O4/c1-4-5-6-7-8-9-12-15-24-20(22)18-13-10-11-14-19(18)21(23)25-16
InchiKey:	JOZQCGPGDCJNNM-UHFFFAOYSA-N
Formula:	C21H38O4
SMILES:	CCCCCCCCCOC(=O)C1CCCCC1C(=O)OCC(C)C
Mol. weight [g/mol]:	354.52

Physical Properties

Property code	Value	Unit	Source
gf	-327.60	kJ/mol	Joback Method
hf	-937.67	kJ/mol	Joback Method
hfus	45.10	kJ/mol	Joback Method
hvap	80.38	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	5.286		Crippen Method
mcvol	310.770	ml/mol	McGowan Method
pc	1139.80	kPa	Joback Method
rinpol	2384.00		NIST Webbook
tb	846.90	K	Joback Method
tc	1044.97	K	Joback Method
tf	458.89	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.42	J/molxK	846.90	Joback Method
cpg	1050.90	J/molxK	879.91	Joback Method
cpg	1068.97	J/molxK	912.92	Joback Method
cpg	1085.66	J/molxK	945.93	Joback Method
cpg	1100.98	J/molxK	978.95	Joback Method
cpg	1114.96	J/molxK	1011.96	Joback Method
cpg	1127.60	J/molxK	1044.97	Joback Method
dvisc	0.0010593	Paxs	458.89	Joback Method
dvisc	0.0004803	Paxs	523.56	Joback Method

dvisc	0.0002591	Paxs	588.23	Joback Method
dvisc	0.0001580	Paxs	652.89	Joback Method
dvisc	0.0001053	Paxs	717.56	Joback Method
dvisc	0.0000751	Paxs	782.23	Joback Method
dvisc	0.0000563	Paxs	846.90	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=U339430&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
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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