

1,2-Cyclohexanedicarboxylic acid, cyclobutyl octyl ester

Inchi:	InChI=1S/C20H34O4/c1-2-3-4-5-6-9-15-23-19(21)17-13-7-8-14-18(17)20(22)24-16-11-10
InchiKey:	FCNXNXWQHSXQOD-UHFFFAOYSA-N
Formula:	C20H34O4
SMILES:	CCCCCCCCOC(=O)C1CCCCC1C(=O)OC1CCC1
Mol. weight [g/mol]:	338.48

Physical Properties

Property code	Value	Unit	Source
gf	-284.93	kJ/mol	Joback Method
hf	-845.11	kJ/mol	Joback Method
hfus	42.07	kJ/mol	Joback Method
hvap	78.63	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.792		Crippen Method
mvol	285.820	ml/mol	McGowan Method
pc	1352.64	kPa	Joback Method
rinpol	2368.00		NIST Webbook
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tb	835.47	K	Joback Method
tc	1041.17	K	Joback Method
tf	477.04	K	Joback Method
vc	1.085	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	958.00	J/molxK	835.47	Joback Method
cpg	1042.16	J/molxK	1006.89	Joback Method
cpg	1028.07	J/molxK	972.61	Joback Method
cpg	1012.64	J/molxK	938.32	Joback Method
cpg	995.84	J/molxK	904.04	Joback Method
cpg	977.64	J/molxK	869.75	Joback Method
cpg	1054.96	J/molxK	1041.17	Joback Method
dvisc	0.0001512	Paxs	835.47	Joback Method

dvisc	0.0001904	Paxs	775.73	Joback Method
dvisc	0.0002493	Paxs	715.99	Joback Method
dvisc	0.0003428	Paxs	656.25	Joback Method
dvisc	0.0005023	Paxs	596.52	Joback Method
dvisc	0.0008015	Paxs	536.78	Joback Method
dvisc	0.0014375	Paxs	477.04	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=U339754&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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