

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

Inchi:	InChI=1S/C20H32O4/c1-2-3-9-14-23-19(21)17-12-7-8-13-18(17)20(22)24-15-16-10-5-4-6
InchiKey:	LHENTQBCOHNCNO-UHFFFAOYSA-N
Formula:	C20H32O4
SMILES:	CCCCCOC(=O)C1CCCCC1C(=O)OCC1CC=CCC1
Mol. weight [g/mol]:	336.47

Physical Properties

Property code	Value	Unit	Source
gf	-279.17	kJ/mol	Joback Method
hf	-799.65	kJ/mol	Joback Method
hfus	39.09	kJ/mol	Joback Method
hvap	79.27	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.426		Crippen Method
mvol	281.520	ml/mol	McGowan Method
pc	1442.44	kPa	Joback Method
rinpol	2414.00		NIST Webbook
rinpol	2414.00		NIST Webbook
tb	843.17	K	Joback Method
tc	1058.14	K	Joback Method
tf	470.76	K	Joback Method
vc	1.054	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	938.36	J/molxK	843.17	Joback Method
cpg	957.90	J/molxK	879.00	Joback Method
cpg	975.77	J/molxK	914.83	Joback Method
cpg	991.99	J/molxK	950.66	Joback Method
cpg	1006.60	J/molxK	986.48	Joback Method
cpg	1019.62	J/molxK	1022.31	Joback Method
cpg	1031.07	J/molxK	1058.14	Joback Method
dvisc	0.0011321	Paxs	470.76	Joback Method

dvisc	0.0005613	Paxs	532.83	Joback Method
dvisc	0.0003222	Paxs	594.90	Joback Method
dvisc	0.0002054	Paxs	656.97	Joback Method
dvisc	0.0001415	Paxs	719.03	Joback Method
dvisc	0.0001034	Paxs	781.10	Joback Method
dvisc	0.0000792	Paxs	843.17	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=U339869&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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