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
mcvol	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	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0005613	Pa×s	532.83	Joback Method
dvisc	0.0003222	Pa×s	594.90	Joback Method
dvisc	0.0002054	Pa×s	656.97	Joback Method
dvisc	0.0001415	Pa×s	719.03	Joback Method
dvisc	0.0001034	Pa×s	781.10	Joback Method
dvisc	0.0000792	Pa×s	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

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