1,2-Cyclohexanedicarboxylic acid, 2-adamantyl ethyl ester

Inchi: InChI=1S/C20H30O4/c1-2-23-19(21)16-5-3-4-6-17(16)20(22)24-18-14-8-12-7-13(10-14)1

InchiKey: YQXLJJRMHPXQEF-UHFFFAOYSA-N

Formula: C20H30O4

SMILES: CCOC(=O)C1CCCCC1C(=O)OC1C2CC3CC(C2)CC1C3

Mol. weight [g/mol]: 334.45

Physical Properties

Property code	Value	Unit	Source
gf	-178.85	kJ/mol	Joback Method
hf	-740.19	kJ/mol	Joback Method
hfus	40.48	kJ/mol	Joback Method
hvap	77.84	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.724		Crippen Method
mcvol	264.100	ml/mol	McGowan Method
pc	1568.47	kPa	Joback Method
rinpol	2478.00		NIST Webbook
rinpol	2478.00		NIST Webbook
tb	839.61	K	Joback Method
tc	1063.14	K	Joback Method
tf	504.44	K	Joback Method
vc	0.997	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	932.56	J/mol×K	839.61	Joback Method
cpg	953.54	J/mol×K	876.86	Joback Method
cpg	972.96	J/mol×K	914.12	Joback Method
cpg	990.89	J/mol×K	951.37	Joback Method
cpg	1007.44	J/mol×K	988.63	Joback Method
cpg	1022.69	J/mol×K	1025.88	Joback Method
cpg	1036.74	J/mol×K	1063.14	Joback Method
dvisc	0.0051580	Pa×s	504.44	Joback Method

dvisc	0.0042521	Pa×s	560.30	Joback Method
dvisc	0.0036302	Pa×s	616.16	Joback Method
dvisc	0.0031818	Pa×s	672.02	Joback Method
dvisc	0.0028458	Pa×s	727.89	Joback Method
dvisc	0.0025861	Pa×s	783.75	Joback Method
dvisc	0.0023802	Pa×s	839.61	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=U339767&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