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

Inchi: InChI=1S/C17H26O4/c1-2-20-16(18)14-10-6-7-11-15(14)17(19)21-12-13-8-4-3-5-9-13/h3

InchiKey: IYQKQGJAPCBFID-UHFFFAOYSA-N

Formula: C17H26O4

SMILES: CCOC(=O)C1CCCCC1C(=O)OCC1CC=CCC1

Mol. weight [g/mol]: 294.39

Physical Properties

Property code	Value	Unit	Source
gf	-304.43	kJ/mol	Joback Method
hf	-737.73	kJ/mol	Joback Method
hfus	31.32	kJ/mol	Joback Method
hvap	72.59	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	3.255		Crippen Method
mcvol	239.250	ml/mol	McGowan Method
pc	1818.50	kPa	Joback Method
rinpol	2127.00		NIST Webbook
rinpol	2127.00		NIST Webbook
tb	774.53	K	Joback Method
tc	996.05	K	Joback Method
tf	436.95	K	Joback Method
vc	0.886	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	759.48	J/mol×K	774.53	Joback Method
cpg	843.60	J/mol×K	959.13	Joback Method
cpg	829.94	J/mol×K	922.21	Joback Method
cpg	814.71	J/mol×K	885.29	Joback Method
cpg	797.90	J/mol×K	848.37	Joback Method
cpg	779.50	J/mol×K	811.45	Joback Method
cpg	855.72	J/mol×K	996.05	Joback Method
dvisc	0.0001177	Pa×s	774.53	Joback Method

dvisc	0.0001524	Pa×s	718.27	Joback Method
dvisc	0.0002062	Pa×s	662.00	Joback Method
dvisc	0.0002949	Pa×s	605.74	Joback Method
dvisc	0.0004541	Pa×s	549.48	Joback Method
dvisc	0.0007715	Pa×s	493.21	Joback Method
dvisc	0.0015023	Pa×s	436.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339866&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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