

1,2-Cyclohexanedicarboxylic acid, ethyl 3-phenylpropyl ester

Inchi:	InChI=1S/C19H26O4/c1-2-22-18(20)16-12-6-7-13-17(16)19(21)23-14-8-11-15-9-4-3-5-10
InchiKey:	KWJDBMFJIKNDEI-UHFFFAOYSA-N
Formula:	C19H26O4
SMILES:	CCOC(=O)C1CCCCC1C(=O)OCCc1ccccc1
Mol. weight [g/mol]:	318.41

Physical Properties

Property code	Value	Unit	Source
gf	-229.59	kJ/mol	Joback Method
hf	-654.58	kJ/mol	Joback Method
hfus	37.49	kJ/mol	Joback Method
hvap	78.60	kJ/mol	Joback Method
log10ws	-4.02		Crippen Method
logp	3.532		Crippen Method
mvol	258.830	ml/mol	McGowan Method
pc	1670.06	kPa	Joback Method
rinpol	2361.00		NIST Webbook
tb	828.26	K	Joback Method
tc	1048.33	K	Joback Method
tf	477.77	K	Joback Method
vc	0.972	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	818.42	J/molxK	828.26	Joback Method
cpg	835.98	J/molxK	864.94	Joback Method
cpg	852.03	J/molxK	901.62	Joback Method
cpg	866.59	J/molxK	938.30	Joback Method
cpg	879.69	J/molxK	974.97	Joback Method
cpg	891.36	J/molxK	1011.65	Joback Method
cpg	901.62	J/molxK	1048.33	Joback Method
dvisc	0.0009434	Paxs	477.77	Joback Method
dvisc	0.0005044	Paxs	536.18	Joback Method

dvisc	0.0003050	Paxs	594.60	Joback Method
dvisc	0.0002018	Paxs	653.01	Joback Method
dvisc	0.0001428	Paxs	711.43	Joback Method
dvisc	0.0001066	Paxs	769.85	Joback Method
dvisc	0.0000829	Paxs	828.26	Joback Method

Sources

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=U339495&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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