

cis-Cyclohex-4-en-1,2-dicarboxylic acid, 3-phenylpropyl propyl ester

Inchi:	InChI=1S/C20H26O4/c1-2-14-23-19(21)17-12-6-7-13-18(17)20(22)24-15-8-11-16-9-4-3-5
InchiKey:	AMPYILGTSIGMAA-UHFFFAOYSA-N
Formula:	C20H26O4
SMILES:	CCCOC(=O)C1CC=CCC1C(=O)OCCc1ccccc1
Mol. weight [g/mol]:	330.42

Physical Properties

Property code	Value	Unit	Source
gf	-191.21	kJ/mol	Joback Method
hf	-617.44	kJ/mol	Joback Method
hfus	41.30	kJ/mol	Joback Method
hvap	81.11	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.698		Crippen Method
mvol	268.620	ml/mol	McGowan Method
pc	1591.08	kPa	Joback Method
rinpol	2433.00		NIST Webbook
rinpol	2433.00		NIST Webbook
tb	850.30	K	Joback Method
tc	1069.77	K	Joback Method
tf	489.80	K	Joback Method
vc	1.014	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	848.95	J/molxK	850.30	Joback Method
cpg	865.67	J/molxK	886.88	Joback Method
cpg	880.90	J/molxK	923.46	Joback Method
cpg	894.67	J/molxK	960.04	Joback Method
cpg	907.02	J/molxK	996.61	Joback Method
cpg	917.98	J/molxK	1033.19	Joback Method
cpg	927.59	J/molxK	1069.77	Joback Method
dvisc	0.0008414	Paxs	489.80	Joback Method

dvisc	0.0004562	Paxs	549.88	Joback Method
dvisc	0.0002790	Paxs	609.97	Joback Method
dvisc	0.0001864	Paxs	670.05	Joback Method
dvisc	0.0001330	Paxs	730.13	Joback Method
dvisc	0.0001000	Paxs	790.22	Joback Method
dvisc	0.0000782	Paxs	850.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382773&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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