1,2-Cyclohexanedicarboxylic acid, 2-cyclohexylethyl ester

Inchi: InChI=1S/C24H40O4/c25-23(27-17-15-19-9-3-1-4-10-19)21-13-7-8-14-22(21)24(26)28-1

InchiKey: YWSMAVGTWOSTET-UHFFFAOYSA-N

Formula: C24H40O4

SMILES: O=C(OCCC1CCCCC1)C1CCCCC1C(=O)OCCC1CCCCC1

Mol. weight [g/mol]: 392.57

Physical Properties

Property code	Value	Unit	Source
gf	-251.00	kJ/mol	Joback Method
hf	-885.67	kJ/mol	Joback Method
hfus	40.07	kJ/mol	Joback Method
hvap	88.31	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	5.820		Crippen Method
mcvol	331.320	ml/mol	McGowan Method
pc	1232.88	kPa	Joback Method
rinpol	2931.00		NIST Webbook
rinpol	2931.00		NIST Webbook
tb	955.08	K	Joback Method
tc	1186.38	K	Joback Method
tf	522.46	K	Joback Method
vc	1.226	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1212.07	J/mol×K	955.08	Joback Method
cpg	1231.45	J/mol×K	993.63	Joback Method
cpg	1248.55	J/mol×K	1032.18	Joback Method
cpg	1263.40	J/mol×K	1070.73	Joback Method
cpg	1276.07	J/mol×K	1109.28	Joback Method
cpg	1286.60	J/mol×K	1147.83	Joback Method
cpg	1295.03	J/mol×K	1186.38	Joback Method
dvisc	0.0008281	Pa×s	522.46	Joback Method

dvisc	0.0003733	Pa×s	594.56	Joback Method
dvisc	0.0002000	Pa×s	666.67	Joback Method
dvisc	0.0001210	Pa×s	738.77	Joback Method
dvisc	0.0000801	Pa×s	810.87	Joback Method
dvisc	0.0000567	Pa×s	882.98	Joback Method
dvisc	0.0000423	Pa×s	955.08	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=U339735&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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