

1,2-Cyclohexanedicarboxylic acid, heptyl methyl ester

Inchi:	InChI=1S/C16H28O4/c1-3-4-5-6-9-12-20-16(18)14-11-8-7-10-13(14)15(17)19-2/h13-14H
InchiKey:	MRYPAFRFFAFHIJ-UHFFFAOYSA-N
Formula:	C16H28O4
SMILES:	CCCCCCCOC(=O)C1CCCCC1C(=O)OC
Mol. weight [g/mol]:	284.39

Physical Properties

Property code	Value	Unit	Source
gf	-367.26	kJ/mol	Joback Method
hf	-829.19	kJ/mol	Joback Method
hfus	35.68	kJ/mol	Joback Method
hvap	69.64	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.479		Crippen Method
mvol	240.320	ml/mol	McGowan Method
pc	1612.88	kPa	Joback Method
rinpol	1977.00		NIST Webbook
rinpol	1977.00		NIST Webbook
tb	732.94	K	Joback Method
tc	929.01	K	Joback Method
tf	417.54	K	Joback Method
vc	0.911	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.43	J/molxK	732.94	Joback Method
cpg	750.19	J/molxK	765.62	Joback Method
cpg	767.80	J/molxK	798.30	Joback Method
cpg	784.28	J/molxK	830.97	Joback Method
cpg	799.62	J/molxK	863.65	Joback Method
cpg	813.84	J/molxK	896.33	Joback Method
cpg	826.93	J/molxK	929.01	Joback Method
dvisc	0.0014656	Paxs	417.54	Joback Method

dvisc	0.0007645	Paxs	470.11	Joback Method
dvisc	0.0004546	Paxs	522.67	Joback Method
dvisc	0.0002972	Paxs	575.24	Joback Method
dvisc	0.0002087	Paxs	627.81	Joback Method
dvisc	0.0001547	Paxs	680.37	Joback Method
dvisc	0.0001198	Paxs	732.94	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=U339654&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

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