

3-Cyclopentylpropionic acid, 4-hexadecyl ester

Inchi:	InChI=1S/C24H46O2/c1-3-5-6-7-8-9-10-11-12-13-19-23(16-4-2)26-24(25)21-20-22-17-14
InchiKey:	FGINXVXCCLZXPY-UHFFFAOYSA-N
Formula:	C24H46O2
SMILES:	CCCCCCCCCCCC(CCC)OC(=O)CCC1CCCC1
Mol. weight [g/mol]:	366.62

Physical Properties

Property code	Value	Unit	Source
gf	-48.61	kJ/mol	Joback Method
hf	-728.29	kJ/mol	Joback Method
hfus	51.11	kJ/mol	Joback Method
hvap	78.04	kJ/mol	Joback Method
log10ws	-8.50		Crippen Method
logp	7.980		Crippen Method
mvol	345.600	ml/mol	McGowan Method
pc	924.99	kPa	Joback Method
rinpol	2473.50		NIST Webbook
rinpol	2473.50		NIST Webbook
tb	839.65	K	Joback Method
tc	1030.80	K	Joback Method
tf	428.30	K	Joback Method
vc	1.339	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1151.76	J/molxK	839.65	Joback Method
cpg	1248.32	J/molxK	998.94	Joback Method
cpg	1231.38	J/molxK	967.09	Joback Method
cpg	1213.29	J/molxK	935.23	Joback Method
cpg	1194.03	J/molxK	903.37	Joback Method
cpg	1173.54	J/molxK	871.51	Joback Method
cpg	1264.18	J/molxK	1030.80	Joback Method
dvisc	0.0000570	Paxs	839.65	Joback Method

dvisc	0.0000774	Paxs	771.09	Joback Method
dvisc	0.0001116	Paxs	702.53	Joback Method
dvisc	0.0001740	Paxs	633.97	Joback Method
dvisc	0.0003023	Paxs	565.42	Joback Method
dvisc	0.0006115	Paxs	496.86	Joback Method
dvisc	0.0015502	Paxs	428.30	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292273&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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