

3-Cyclopentylpropionic acid, pentadecyl ester

Inchi:	InChI=1S/C23H44O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-21-25-23(24)20-19-22-17-14-15
InchiKey:	NGRWBWMGWJUELO-UHFFFAOYSA-N
Formula:	C23H44O2
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCC1CCCC1
Mol. weight [g/mol]:	352.59

Physical Properties

Property code	Value	Unit	Source
gf	-54.59	kJ/mol	Joback Method
hf	-702.37	kJ/mol	Joback Method
hfus	52.05	kJ/mol	Joback Method
hvap	76.20	kJ/mol	Joback Method
log10ws	-7.97		Crippen Method
logp	7.591		Crippen Method
mvol	331.510	ml/mol	McGowan Method
pc	976.56	kPa	Joback Method
rinpol	2532.70		NIST Webbook
rinpol	2532.70		NIST Webbook
tb	817.21	K	Joback Method
tc	1004.78	K	Joback Method
tf	432.03	K	Joback Method
vc	1.288	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1088.00	J/molxK	817.21	Joback Method
cpg	1109.39	J/molxK	848.47	Joback Method
cpg	1129.57	J/molxK	879.73	Joback Method
cpg	1148.59	J/molxK	910.99	Joback Method
cpg	1166.48	J/molxK	942.25	Joback Method
cpg	1183.30	J/molxK	973.52	Joback Method
cpg	1199.08	J/molxK	1004.78	Joback Method
dvisc	0.0014458	Paxs	432.03	Joback Method

dvisc	0.0006336	Paxs	496.23	Joback Method
dvisc	0.0003354	Paxs	560.42	Joback Method
dvisc	0.0002024	Paxs	624.62	Joback Method
dvisc	0.0001341	Paxs	688.82	Joback Method
dvisc	0.0000954	Paxs	753.01	Joback Method
dvisc	0.0000716	Paxs	817.21	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292339&Units=SI

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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