

3-Cyclopentylpropionic acid, octyl ester

Inchi:	InChI=1S/C16H30O2/c1-2-3-4-5-6-9-14-18-16(17)13-12-15-10-7-8-11-15/h15H,2-14H2,1
InchiKey:	AHSRJCSVGJRRDQ-UHFFFAOYSA-N
Formula:	C16H30O2
SMILES:	CCCCCCCCOC(=O)CCC1CCCC1
Mol. weight [g/mol]:	254.41

Physical Properties

Property code	Value	Unit	Source
gf	-113.53	kJ/mol	Joback Method
hf	-557.89	kJ/mol	Joback Method
hfus	33.92	kJ/mol	Joback Method
hvap	60.62	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.861		Crippen Method
mvol	232.880	ml/mol	McGowan Method
pc	1564.75	kPa	Joback Method
rinpol	1848.30		NIST Webbook
tb	657.05	K	Joback Method
tc	842.14	K	Joback Method
tf	353.14	K	Joback Method
vc	0.896	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	667.99	J/molxK	657.05	Joback Method
cpg	687.70	J/molxK	687.90	Joback Method
cpg	706.41	J/molxK	718.75	Joback Method
cpg	724.15	J/molxK	749.60	Joback Method
cpg	740.94	J/molxK	780.45	Joback Method
cpg	756.82	J/molxK	811.30	Joback Method
cpg	771.81	J/molxK	842.14	Joback Method
dvisc	0.0027008	Paxs	353.14	Joback Method
dvisc	0.0012827	Paxs	403.79	Joback Method

dvisc	0.0007192	Paxs	454.44	Joback Method
dvisc	0.0004528	Paxs	505.09	Joback Method
dvisc	0.0003102	Paxs	555.75	Joback Method
dvisc	0.0002264	Paxs	606.40	Joback Method
dvisc	0.0001734	Paxs	657.05	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=U292335&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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