

Tetracosyl cyclopentanecarboxylate

Inchi: InChI=1S/C30H58O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-25-28
InchiKey: AIUDCZYSBALPBE-UHFFFAOYSA-N
Formula: C30H58O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCOC(=O)C1CCCC1
Mol. weight [g/mol]: 450.78

Physical Properties

Property code	Value	Unit	Source
gf	4.35	kJ/mol	Joback Method
hf	-846.85	kJ/mol	Joback Method
hfus	70.18	kJ/mol	Joback Method
hvap	91.79	kJ/mol	Joback Method
log10ws	-10.90		Crippen Method
logp	10.322		Crippen Method
mvol	430.140	ml/mol	McGowan Method
pc	667.01	kPa	Joback Method
rinpol	3233.30		NIST Webbook
rinpol	3233.30		NIST Webbook
tb	977.37	K	Joback Method
tc	1204.50	K	Joback Method
tf	510.92	K	Joback Method
vc	1.681	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1542.90	J/molxK	977.37	Joback Method
cpg	1649.35	J/molxK	1166.64	Joback Method
cpg	1631.23	J/molxK	1128.79	Joback Method
cpg	1611.64	J/molxK	1090.93	Joback Method
cpg	1590.45	J/molxK	1053.08	Joback Method
cpg	1567.57	J/molxK	1015.22	Joback Method
cpg	1666.08	J/molxK	1204.50	Joback Method
dvisc	0.0000257	Paxs	977.37	Joback Method

dvisc	0.0000347	Paxs	899.63	Joback Method
dvisc	0.0000497	Paxs	821.89	Joback Method
dvisc	0.0000767	Paxs	744.14	Joback Method
dvisc	0.0001310	Paxs	666.40	Joback Method
dvisc	0.0002577	Paxs	588.66	Joback Method
dvisc	0.0006229	Paxs	510.92	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=U412784&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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