

Cyclohexyl heptadecanoate

Inchi:	InChI=1S/C23H44O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-18-21-23(24)25-22-19-16-15-17
InchiKey:	AGQQDRCCFNAEBC-UHFFFAOYSA-N
Formula:	C23H44O2
SMILES:	CCCCCCCCCCCCCCCC(=O)OC1CCCCC1
Mol. weight [g/mol]:	352.59

Physical Properties

Property code	Value	Unit	Source
gf	-66.69	kJ/mol	Joback Method
hf	-708.53	kJ/mol	Joback Method
hfus	49.95	kJ/mol	Joback Method
hvap	76.38	kJ/mol	Joback Method
log10ws	-8.32		Crippen Method
logp	7.734		Crippen Method
mvol	331.510	ml/mol	McGowan Method
pc	992.00	kPa	Joback Method
rinpol	2523.00		NIST Webbook
rinpol	2523.00		NIST Webbook
tb	821.48	K	Joback Method
tc	1011.43	K	Joback Method
tf	428.51	K	Joback Method
vc	1.280	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1092.72	J/molxK	821.48	Joback Method
cpg	1114.37	J/molxK	853.14	Joback Method
cpg	1134.73	J/molxK	884.80	Joback Method
cpg	1153.83	J/molxK	916.46	Joback Method
cpg	1171.72	J/molxK	948.11	Joback Method
cpg	1188.43	J/molxK	979.77	Joback Method
cpg	1204.01	J/molxK	1011.43	Joback Method
dvisc	0.0013771	Paxs	428.51	Joback Method

dvisc	0.0005496	Paxs	494.00	Joback Method
dvisc	0.0002720	Paxs	559.50	Joback Method
dvisc	0.0001560	Paxs	625.00	Joback Method
dvisc	0.0000994	Paxs	690.49	Joback Method
dvisc	0.0000685	Paxs	755.99	Joback Method
dvisc	0.0000501	Paxs	821.48	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=R541498&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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