

Octacosan-14-one

Inchi:	InChI=1S/C28H56O/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-28(29)26-24-22-20-18-16-1
InchiKey:	DBADHDAADPVAEV-UHFFFAOYSA-N
Formula:	C28H56O
SMILES:	CCCCCCCCCCCCCCCC(=O)CCCCCCCCCCCC
Mol. weight [g/mol]:	408.74
CAS:	31815-02-8

Physical Properties

Property code	Value	Unit	Source
gf	55.96	kJ/mol	Joback Method
hf	-733.83	kJ/mol	Joback Method
hfus	69.88	kJ/mol	Joback Method
hvap	84.67	kJ/mol	Joback Method
log10ws	-10.82		Crippen Method
logp	10.348		Crippen Method
mvol	406.950	ml/mol	McGowan Method
pc	677.11	kPa	Joback Method
rinpol	2988.90		NIST Webbook
rinpol	2988.90		NIST Webbook
tb	893.91	K	Joback Method
tc	1098.64	K	Joback Method
tf	455.25	K	Joback Method
vc	1.609	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1381.36	J/mol×K	893.91	Joback Method
cpg	1405.83	J/mol×K	928.03	Joback Method
cpg	1428.89	J/mol×K	962.15	Joback Method
cpg	1450.60	J/mol×K	996.28	Joback Method
cpg	1471.05	J/mol×K	1030.40	Joback Method
cpg	1490.30	J/mol×K	1064.52	Joback Method
cpg	1508.42	J/mol×K	1098.64	Joback Method

dvisc	0.0009703	Paxs	455.25	Joback Method
dvisc	0.0003676	Paxs	528.36	Joback Method
dvisc	0.0001763	Paxs	601.47	Joback Method
dvisc	0.0000992	Paxs	674.58	Joback Method
dvisc	0.0000624	Paxs	747.69	Joback Method
dvisc	0.0000427	Paxs	820.80	Joback Method
dvisc	0.0000311	Paxs	893.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31815028&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
mvol:	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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