Hexacosyl cyclopentanecarboxylate

Inchi: InChI=1S/C32H62O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24
InchiKey: KRBCQUXULQKNPL-UHFFFAOYSA-N
Formula: C32H62O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCOC(=O)C1CCCC1
Mol. weight [g/mol]: 478.83

Physical Properties

Property code	Value	Unit	Source
gf	21.19	kJ/mol	Joback Method
hf	-888.13	kJ/mol	Joback Method
hfus	75.36	kJ/mol	Joback Method
hvap	96.24	kJ/mol	Joback Method
log10ws	-11.73		Crippen Method
logp	11.102		Crippen Method
mcvol	458.320	ml/mol	McGowan Method
pc	605.47	kPa	Joback Method
rinpol	3439.30		NIST Webbook
rinpol	3439.30		NIST Webbook
tb	1023.13	K	Joback Method
tc	1271.82	K	Joback Method
tf	533.46	K	Joback Method
vc	1.792	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1676.67	J/mol×K	1023.13	Joback Method
cpg	1788.36	J/mol×K	1230.37	Joback Method
cpg	1769.64	J/mol×K	1188.92	Joback Method
cpg	1749.26	J/mol×K	1147.47	Joback Method
cpg	1727.07	J/mol×K	1106.03	Joback Method
cpg	1702.92	J/mol×K	1064.58	Joback Method
cpg	1805.57	J/mol×K	1271.82	Joback Method
dvisc	0.0000188	Pa×s	1023.13	Joback Method

dvisc	0.0000255	Pa×s	941.52	Joback Method
dvisc	0.0000367	Pa×s	859.91	Joback Method
dvisc	0.0000570	Pa×s	778.30	Joback Method
dvisc	0.0000980	Pa×s	696.68	Joback Method
dvisc	0.0001947	Pa×s	615.07	Joback Method
dvisc	0.0004770	Pa×s	533.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U412785&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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