

propyl octacosanoate

Inchi: InChI=1S/C31H62O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-25
InchiKey: UKEGCRCBZWNJKU-UHFFFAOYSA-N
Formula: C31H62O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCC(=O)OCC
Mol. weight [g/mol]: 466.82

Physical Properties

Property code	Value	Unit	Source
gf	-23.78	kJ/mol	Joback Method
hf	-927.97	kJ/mol	Joback Method
hfus	78.83	kJ/mol	Joback Method
hvap	93.76	kJ/mol	Joback Method
log10ws	-11.66		Crippen Method
logp	11.102		Crippen Method
mcvol	455.090	ml/mol	McGowan Method
pc	581.20	kPa	Joback Method
rinpol	3278.46		NIST Webbook
tb	984.97	K	Joback Method
tc	1231.24	K	Joback Method
tf	511.29	K	Joback Method
vc	1.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1615.90	J/molxK	984.97	Joback Method
cpg	1643.25	J/molxK	1026.01	Joback Method
cpg	1668.49	J/molxK	1067.06	Joback Method
cpg	1691.73	J/molxK	1108.10	Joback Method
cpg	1713.09	J/molxK	1149.15	Joback Method
cpg	1732.71	J/molxK	1190.19	Joback Method
cpg	1750.69	J/molxK	1231.24	Joback Method
dvisc	0.0004241	Paxs	511.29	Joback Method
dvisc	0.0001655	Paxs	590.24	Joback Method

dvisc	0.0000806	Paxs	669.18	Joback Method
dvisc	0.0000457	Paxs	748.13	Joback Method
dvisc	0.0000289	Paxs	827.08	Joback Method
dvisc	0.0000198	Paxs	906.02	Joback Method
dvisc	0.0000144	Paxs	984.97	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=R438025&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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