

decyl docosanoate

Inchi:	InChI=1S/C32H64O2/c1-3-5-7-9-11-13-14-15-16-17-18-19-20-21-22-23-24-26-28-30-32(
InchiKey:	KSCAZGPKPGSMTR-UHFFFAOYSA-N
Formula:	C32H64O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCC(=O)OCCCCCCCCC
Mol. weight [g/mol]:	480.85
CAS:	42218-29-1

Physical Properties

Property code	Value	Unit	Source
gf	-15.36	kJ/mol	Joback Method
hf	-948.61	kJ/mol	Joback Method
hfus	81.42	kJ/mol	Joback Method
hvap	95.98	kJ/mol	Joback Method
log10ws	-12.08		Crippen Method
logp	11.492		Crippen Method
mcvol	469.180	ml/mol	McGowan Method
pc	555.20	kPa	Joback Method
rinpol	3354.63		NIST Webbook
tb	1007.85	K	Joback Method
tc	1268.18	K	Joback Method
tf	522.56	K	Joback Method
vc	1.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1683.18	J/molxK	1007.85	Joback Method
cpg	1803.68	J/molxK	1224.79	Joback Method
cpg	1783.67	J/molxK	1181.40	Joback Method
cpg	1761.76	J/molxK	1138.01	Joback Method
cpg	1737.81	J/molxK	1094.63	Joback Method
cpg	1711.67	J/molxK	1051.24	Joback Method
cpg	1821.94	J/molxK	1268.18	Joback Method
dvisc	0.0000123	Paxs	1007.85	Joback Method

dvisc	0.0000169	Paxs	926.97	Joback Method
dvisc	0.0000247	Paxs	846.09	Joback Method
dvisc	0.0000392	Paxs	765.20	Joback Method
dvisc	0.0000693	Paxs	684.32	Joback Method
dvisc	0.0001429	Paxs	603.44	Joback Method
dvisc	0.0003683	Paxs	522.56	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=C42218291&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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