

hexyl docosanoate

Inchi:	InChI=1S/C28H56O2/c1-3-5-7-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-26-28(
InchiKey:	SZHHTCPIUIMTIX-UHFFFAOYSA-N
Formula:	C28H56O2
SMILES:	CCCCCCCCCCCCCCCCCCCC(=O)OCCCCC
Mol. weight [g/mol]:	424.74
CAS:	26720-37-6

Physical Properties

Property code	Value	Unit	Source
gf	-49.04	kJ/mol	Joback Method
hf	-866.05	kJ/mol	Joback Method
hfus	71.06	kJ/mol	Joback Method
hvap	87.08	kJ/mol	Joback Method
log10ws	-10.41		Crippen Method
logp	9.932		Crippen Method
mvol	412.820	ml/mol	McGowan Method
pc	671.16	kPa	Joback Method
rinpol	2966.35		NIST Webbook
rinpol	2966.35		NIST Webbook
tb	916.33	K	Joback Method
tc	1129.21	K	Joback Method
tf	477.48	K	Joback Method
vc	1.627	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1416.23	J/molxK	916.33	Joback Method
cpg	1440.70	J/molxK	951.81	Joback Method
cpg	1463.57	J/molxK	987.29	Joback Method
cpg	1484.93	J/molxK	1022.77	Joback Method
cpg	1504.83	J/molxK	1058.25	Joback Method
cpg	1523.34	J/molxK	1093.73	Joback Method
cpg	1540.54	J/molxK	1129.21	Joback Method

dvisc	0.0006385	Paxs	477.48	Joback Method
dvisc	0.0002539	Paxs	550.62	Joback Method
dvisc	0.0001253	Paxs	623.76	Joback Method
dvisc	0.0000717	Paxs	696.90	Joback Method
dvisc	0.0000457	Paxs	770.05	Joback Method
dvisc	0.0000314	Paxs	843.19	Joback Method
dvisc	0.0000230	Paxs	916.33	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=C26720376&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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