

Eicosanyl formate

Inchi:	InChI=1S/C21H42O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-23-21-22/h2
InchiKey:	XPSVNIWOCPFNFQ-UHFFFAOYSA-N
Formula:	C21H42O2
SMILES:	CCCCCCCCCCCCCCCCCCCCOC=O
Mol. weight [g/mol]:	326.56

Physical Properties

Property code	Value	Unit	Source
gf	-78.58	kJ/mol	Joback Method
hf	-694.57	kJ/mol	Joback Method
hfus	53.62	kJ/mol	Joback Method
hvap	71.47	kJ/mol	Joback Method
log10ws	-7.48		Crippen Method
logp	7.201		Crippen Method
mcvol	314.190	ml/mol	McGowan Method
pc	990.75	kPa	Joback Method
rmpol	2323.00		NIST Webbook
tb	750.96	K	Joback Method
tc	922.75	K	Joback Method
tf	390.66	K	Joback Method
vc	1.246	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	967.84	J/molxK	750.96	Joback Method
cpg	987.82	J/molxK	779.59	Joback Method
cpg	1006.87	J/molxK	808.22	Joback Method
cpg	1024.99	J/molxK	836.86	Joback Method
cpg	1042.23	J/molxK	865.49	Joback Method
cpg	1058.60	J/molxK	894.12	Joback Method
cpg	1074.12	J/molxK	922.75	Joback Method
dvisc	0.0017458	Paxs	390.66	Joback Method
dvisc	0.0007187	Paxs	450.71	Joback Method

dvisc	0.0003645	Paxs	510.76	Joback Method
dvisc	0.0002133	Paxs	570.81	Joback Method
dvisc	0.0001382	Paxs	630.86	Joback Method
dvisc	0.0000965	Paxs	690.91	Joback Method
dvisc	0.0000714	Paxs	750.96	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=R543003&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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