

eicosanyl docosanoate

Other names:	icosyl docosanoate
Inchi:	InChI=1S/C42H84O2/c1-3-5-7-9-11-13-15-17-19-21-23-24-26-28-30-32-34-36-38-40-42(
InchiKey:	JWEYEHAVGPUUDR-UHFFFAOYSA-N
Formula:	C42H84O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCC(=O)OCCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	621.12
CAS:	42233-14-7

Physical Properties

Property code	Value	Unit	Source
gf	68.84	kJ/mol	Joback Method
hf	-1155.01	kJ/mol	Joback Method
hfus	107.32	kJ/mol	Joback Method
hvap	118.24	kJ/mol	Joback Method
log10ws	-16.27		Crippen Method
logp	15.393		Crippen Method
mcvol	610.080	ml/mol	McGowan Method
pc	369.25	kPa	Joback Method
rinpol	4346.38		NIST Webbook
tb	1236.65	K	Joback Method
tc	1759.52	K	Joback Method
tf	635.26	K	Joback Method
vc	2.412	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2367.68	J/molxK	1236.65	Joback Method
cpg	2550.10	J/molxK	1672.38	Joback Method
cpg	2520.37	J/molxK	1585.23	Joback Method
cpg	2488.95	J/molxK	1498.09	Joback Method
cpg	2454.15	J/molxK	1410.94	Joback Method
cpg	2414.29	J/molxK	1323.80	Joback Method
cpg	2579.83	J/molxK	1759.52	Joback Method

dvisc	0.0000024	Paxs	1236.65	Joback Method
dvisc	0.0000033	Paxs	1136.42	Joback Method
dvisc	0.0000049	Paxs	1036.19	Joback Method
dvisc	0.0000079	Paxs	935.96	Joback Method
dvisc	0.0000142	Paxs	835.72	Joback Method
dvisc	0.0000303	Paxs	735.49	Joback Method
dvisc	0.0000818	Paxs	635.26	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C42233147&Units=SI

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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