

Fumaric acid, di(tetradec-3-enyl) ester

Inchi: InChI=1S/C32H56O4/c1-3-5-7-9-11-13-15-17-19-21-23-25-29-35-31(33)27-28-32(34)36-
InchiKey: XIBFVAYWVIZSPB-RKDWFBATSA-N
Formula: C32H56O4
SMILES: CCCCCCCCCC=CCCOC(=O)C=CC(=O)OCCC=CCCCCCCCCCC
Mol. weight [g/mol]: 504.78

Physical Properties

Property code	Value	Unit	Source
gf	-8.62	kJ/mol	Joback Method
hf	-841.75	kJ/mol	Joback Method
hfus	84.82	kJ/mol	Joback Method
hvap	105.01	kJ/mol	Joback Method
log10ws	-10.50		Crippen Method
logp	9.583		Crippen Method
mvol	463.720	ml/mol	McGowan Method
pc	612.08	kPa	Joback Method
rinpol	3620.00		NIST Webbook
rinpol	3620.00		NIST Webbook
tb	1096.62	K	Joback Method
tc	1379.82	K	Joback Method
tf	579.48	K	Joback Method
vc	1.815	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1652.05	J/molxK	1096.62	Joback Method
cpg	1764.22	J/molxK	1332.62	Joback Method
cpg	1744.30	J/molxK	1285.42	Joback Method
cpg	1723.36	J/molxK	1238.22	Joback Method
cpg	1701.17	J/molxK	1191.02	Joback Method
cpg	1677.48	J/molxK	1143.82	Joback Method
cpg	1783.36	J/molxK	1379.82	Joback Method
dvisc	0.0000057	Paxs	1096.62	Joback Method

dvisc	0.0000077	Paxs	1010.43	Joback Method
dvisc	0.0000112	Paxs	924.24	Joback Method
dvisc	0.0000174	Paxs	838.05	Joback Method
dvisc	0.0000301	Paxs	751.86	Joback Method
dvisc	0.0000597	Paxs	665.67	Joback Method
dvisc	0.0001456	Paxs	579.48	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=U348845&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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