

Fumaric acid, dec-4-enyl octadecyl ester

Inchi:	InChI=1S/C32H58O4/c1-3-5-7-9-11-13-14-15-16-17-18-19-20-22-24-26-30-36-32(34)28-
InchiKey:	KHIDZLVZWLMZTJ-KQHZTYPXSA-N
Formula:	C32H58O4
SMILES:	CCCCC=CCCCOC(=O)C=CC(=O)OCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]:	506.80

Physical Properties

Property code	Value	Unit	Source
gf	-88.84	kJ/mol	Joback Method
hf	-958.97	kJ/mol	Joback Method
hfus	84.61	kJ/mol	Joback Method
hvap	105.05	kJ/mol	Joback Method
log10ws	-10.65		Crippen Method
logp	9.807		Crippen Method
mvol	468.020	ml/mol	McGowan Method
pc	596.63	kPa	Joback Method
rinpol	3598.00		NIST Webbook
rinpol	3598.00		NIST Webbook
tb	1092.46	K	Joback Method
tc	1381.03	K	Joback Method
tf	584.56	K	Joback Method
vc	1.835	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1680.26	J/molxK	1092.46	Joback Method
cpg	1788.50	J/molxK	1332.94	Joback Method
cpg	1770.33	J/molxK	1284.84	Joback Method
cpg	1750.65	J/molxK	1236.75	Joback Method
cpg	1729.22	J/molxK	1188.65	Joback Method
cpg	1705.83	J/molxK	1140.56	Joback Method
cpg	1805.39	J/molxK	1381.03	Joback Method
dvisc	0.0000064	Paxs	1092.46	Joback Method

dvisc	0.0000088	Paxs	1007.81	Joback Method
dvisc	0.0000126	Paxs	923.16	Joback Method
dvisc	0.0000196	Paxs	838.51	Joback Method
dvisc	0.0000335	Paxs	753.86	Joback Method
dvisc	0.0000656	Paxs	669.21	Joback Method
dvisc	0.0001563	Paxs	584.56	Joback Method

Sources

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=U348952&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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