

Fumaric acid, 3-hexyl octadecyl ester

Inchi: InChI=1S/C28H52O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-25-31-27(29)23-
InchiKey: AAIUMAFAHOTZCY-WCWDXBQESA-N
Formula: C28H52O4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(CC)CCC
Mol. weight [g/mol]: 452.71

Physical Properties

Property code	Value	Unit	Source
gf	-205.18	kJ/mol	Joback Method
hf	-998.91	kJ/mol	Joback Method
hfus	70.53	kJ/mol	Joback Method
hvap	95.80	kJ/mol	Joback Method
log10ws	-9.23		Crippen Method
logp	8.469		Crippen Method
mvol	415.960	ml/mol	McGowan Method
pc	709.60	kPa	Joback Method
rinpol	3092.00		NIST Webbook
rinpol	3092.00		NIST Webbook
tb	996.34	K	Joback Method
tc	1231.91	K	Joback Method
tf	529.56	K	Joback Method
vc	1.625	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1446.75	J/molxK	996.34	Joback Method
cpg	1468.66	J/molxK	1035.60	Joback Method
cpg	1488.79	J/molxK	1074.86	Joback Method
cpg	1507.22	J/molxK	1114.12	Joback Method
cpg	1524.05	J/molxK	1153.39	Joback Method
cpg	1539.36	J/molxK	1192.65	Joback Method
cpg	1553.25	J/molxK	1231.91	Joback Method
dvisc	0.0003320	Paxs	529.56	Joback Method

dvisc	0.0001357	Paxs	607.36	Joback Method
dvisc	0.0000680	Paxs	685.15	Joback Method
dvisc	0.0000392	Paxs	762.95	Joback Method
dvisc	0.0000250	Paxs	840.75	Joback Method
dvisc	0.0000173	Paxs	918.54	Joback Method
dvisc	0.0000126	Paxs	996.34	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=U348616&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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