

Fumaric acid, 2-heptyl octadecyl ester

Inchi:	InChI=1S/C29H54O4/c1-4-6-8-9-10-11-12-13-14-15-16-17-18-19-20-22-26-32-28(30)24-
InchiKey:	WSRUVBRJYDQFCT-OCOZRVBESA-N
Formula:	C29H54O4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)CCCC
Mol. weight [g/mol]:	466.74

Physical Properties

Property code	Value	Unit	Source
gf	-196.76	kJ/mol	Joback Method
hf	-1019.55	kJ/mol	Joback Method
hfus	73.12	kJ/mol	Joback Method
hvap	98.03	kJ/mol	Joback Method
log10ws	-9.65		Crippen Method
logp	8.859		Crippen Method
mcvol	430.050	ml/mol	McGowan Method
pc	674.65	kPa	Joback Method
rinqol	3196.00		NIST Webbook
tb	1019.22	K	Joback Method
tc	1266.06	K	Joback Method
tf	540.83	K	Joback Method
vc	1.681	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1511.74	J/molxK	1019.22	Joback Method
cpg	1606.58	J/molxK	1224.92	Joback Method
cpg	1591.09	J/molxK	1183.78	Joback Method
cpg	1573.97	J/molxK	1142.64	Joback Method
cpg	1555.11	J/molxK	1101.50	Joback Method
cpg	1534.40	J/molxK	1060.36	Joback Method
cpg	1620.54	J/molxK	1266.06	Joback Method
dvisc	0.0000107	Paxs	1019.22	Joback Method
dvisc	0.0000147	Paxs	939.49	Joback Method

dvisc	0.0000214	Paxs	859.76	Joback Method
dvisc	0.0000336	Paxs	780.02	Joback Method
dvisc	0.0000585	Paxs	700.29	Joback Method
dvisc	0.0001173	Paxs	620.56	Joback Method
dvisc	0.0002886	Paxs	540.83	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=U348635&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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