

Fumaric acid, heptyl 3-hexyl ester

Inchi:	InChI=1S/C17H30O4/c1-4-7-8-9-10-14-20-16(18)12-13-17(19)21-15(6-3)11-5-2/h12-13,1
InchiKey:	HDGRXVNFQBQPMR-OUKQBFOZSA-N
Formula:	C17H30O4
SMILES:	CCCCCCCOC(=O)C=CC(=O)OC(CC)CCC
Mol. weight [g/mol]:	298.42

Physical Properties

Property code	Value	Unit	Source
gf	-297.80	kJ/mol	Joback Method
hf	-771.87	kJ/mol	Joback Method
hfus	42.04	kJ/mol	Joback Method
hvap	71.32	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.178		Crippen Method
mcvol	260.970	ml/mol	McGowan Method
pc	1373.78	kPa	Joback Method
rinsol	1993.00		NIST Webbook
tb	744.66	K	Joback Method
tc	927.57	K	Joback Method
tf	405.59	K	Joback Method
vc	1.010	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.78	J/molxK	744.66	Joback Method
cpg	784.43	J/molxK	775.14	Joback Method
cpg	800.20	J/molxK	805.63	Joback Method
cpg	815.12	J/molxK	836.11	Joback Method
cpg	829.19	J/molxK	866.60	Joback Method
cpg	842.44	J/molxK	897.08	Joback Method
cpg	854.89	J/molxK	927.57	Joback Method
dvisc	0.0012840	Paxs	405.59	Joback Method
dvisc	0.0005755	Paxs	462.10	Joback Method

dvisc	0.0003072	Paxs	518.61	Joback Method
dvisc	0.0001855	Paxs	575.12	Joback Method
dvisc	0.0001226	Paxs	631.64	Joback Method
dvisc	0.0000868	Paxs	688.15	Joback Method
dvisc	0.0000647	Paxs	744.66	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=U348606&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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