

Fumaric acid, ethyl 3-heptyl ester

Inchi:	InChI=1S/C13H22O4/c1-4-7-8-11(5-2)17-13(15)10-9-12(14)16-6-3/h9-11H,4-8H2,1-3H3
InchiKey:	MXJFIXKMCXINGU-MDZDMXLPSA-N
Formula:	C13H22O4
SMILES:	CCCCC(CC)OC(=O)C=CC(=O)OCC
Mol. weight [g/mol]:	242.31

Physical Properties

Property code	Value	Unit	Source
gf	-331.48	kJ/mol	Joback Method
hf	-689.31	kJ/mol	Joback Method
hfus	31.68	kJ/mol	Joback Method
hvap	62.41	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.618		Crippen Method
mcvol	204.610	ml/mol	McGowan Method
pc	1867.55	kPa	Joback Method
rinsol	1581.00		NIST Webbook
tb	653.14	K	Joback Method
tc	838.21	K	Joback Method
tf	360.51	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.34	J/molxK	653.14	Joback Method
cpg	614.70	J/molxK	807.36	Joback Method
cpg	602.64	J/molxK	776.52	Joback Method
cpg	589.89	J/molxK	745.67	Joback Method
cpg	576.43	J/molxK	714.83	Joback Method
cpg	562.25	J/molxK	683.98	Joback Method
cpg	626.08	J/molxK	838.21	Joback Method
dvisc	0.0001079	Paxs	653.14	Joback Method
dvisc	0.0001431	Paxs	604.37	Joback Method

dvisc	0.0001995	Paxs	555.60	Joback Method
dvisc	0.0002963	Paxs	506.82	Joback Method
dvisc	0.0004789	Paxs	458.05	Joback Method
dvisc	0.0008679	Paxs	409.28	Joback Method
dvisc	0.0018471	Paxs	360.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348677&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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