Fumaric acid, 3-heptyl hexyl ester

Inchi: InChI=1S/C17H30O4/c1-4-7-9-10-14-20-16(18)12-13-17(19)21-15(6-3)11-8-5-2/h12-13,1
InchiKey: XAUUQIKPJURQKO-OUKQBFOZSA-N
Formula: C17H30O4
SMILES: CCCCCCOC(=O)C=CC(=O)OC(CC)CCCC
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
rinpol	1995.00		NIST Webbook
rinpol	1995.00		NIST Webbook
tb	744.66	K	Joback Method
tc	927.57	K	Joback Method
tf	405.59	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.78	J/mol×K	744.66	Joback Method
cpg	842.44	J/mol×K	897.08	Joback Method
cpg	829.19	J/mol×K	866.60	Joback Method
cpg	815.12	J/mol×K	836.11	Joback Method
cpg	800.20	J/mol×K	805.63	Joback Method
cpg	784.43	J/mol×K	775.14	Joback Method
cpg	854.89	J/mol×K	927.57	Joback Method
dvisc	0.0000647	Pa×s	744.66	Joback Method

dvisc	0.0000868	Pa×s	688.15	Joback Method
dvisc	0.0001226	Pa×s	631.64	Joback Method
dvisc	0.0001855	Pa×s	575.12	Joback Method
dvisc	0.0003072	Pa×s	518.61	Joback Method
dvisc	0.0005755	Pa×s	462.10	Joback Method
dvisc	0.0012840	Pa×s	405.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348683&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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