Fumaric acid, ethyl 4-heptyl ester

Inchi: InChI=1S/C13H22O4/c1-4-7-11(8-5-2)17-13(15)10-9-12(14)16-6-3/h9-11H,4-8H2,1-3H3/
InchiKey: DYMCTBBMZSGDAR-MDZDMXLPSA-N
Formula: C13H22O4
SMILES: CCCC(CCC)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
rinpol	1574.00		NIST Webbook
rinpol	1574.00		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/mol×K	653.14	Joback Method
cpg	562.25	J/mol×K	683.98	Joback Method
cpg	576.43	J/mol×K	714.83	Joback Method
cpg	589.89	J/mol×K	745.67	Joback Method
cpg	602.64	J/mol×K	776.52	Joback Method
cpg	614.70	J/mol×K	807.36	Joback Method
cpg	626.08	J/mol×K	838.21	Joback Method
dvisc	0.0018471	Pa×s	360.51	Joback Method

dvisc	0.0008679	Pa×s	409.28	Joback Method
dvisc	0.0004789	Pa×s	458.05	Joback Method
dvisc	0.0002963	Pa×s	506.82	Joback Method
dvisc	0.0001995	Pa×s	555.60	Joback Method
dvisc	0.0001431	Pa×s	604.37	Joback Method
dvisc	0.0001079	Pa×s	653.14	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U348512&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