Fumaric acid, 2-heptyl propyl ester

Inchi: InChI=1S/C14H24O4/c1-4-6-7-8-12(3)18-14(16)10-9-13(15)17-11-5-2/h9-10,12H,4-8,11H
InchiKey: BITHVIZMCVRERN-MDZDMXLPSA-N
Formula: C14H24O4
SMILES: CCCCCC(C)OC(=O)C=CC(=O)OCCC
Mol. weight [g/mol]: 256.34

Physical Properties

Property code	Value	Unit	Source
gf	-323.06	kJ/mol	Joback Method
hf	-709.95	kJ/mol	Joback Method
hfus	34.27	kJ/mol	Joback Method
hvap	64.64	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.008		Crippen Method
mcvol	218.700	ml/mol	McGowan Method
pc	1721.73	kPa	Joback Method
rinpol	1708.00		NIST Webbook
tb	676.02	K	Joback Method
tc	859.88	K	Joback Method
tf	371.78	K	Joback Method
vc	0.842	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.60	J/mol×K	676.02	Joback Method
cpg	616.00	J/mol×K	706.66	Joback Method
cpg	630.64	J/mol×K	737.31	Joback Method
cpg	644.52	J/mol×K	767.95	Joback Method
cpg	657.67	J/mol×K	798.59	Joback Method
cpg	670.09	J/mol×K	829.24	Joback Method
cpg	681.79	J/mol×K	859.88	Joback Method
dvisc	0.0017024	Pa×s	371.78	Joback Method
dvisc	0.0007897	Pa×s	422.49	Joback Method

dvisc	0.0004319	Pa×s	473.19	Joback Method
dvisc	0.0002655	Pa×s	523.90	Joback Method
dvisc	0.0001778	Pa×s	574.61	Joback Method
dvisc	0.0001271	Pa×s	625.31	Joback Method
dvisc	0.0000955	Pa×s	676.02	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348621&Units=SI

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