Fumaric acid, 3-heptyl isobutyl ester

Inchi: InChI=1S/C15H26O4/c1-5-7-8-13(6-2)19-15(17)10-9-14(16)18-11-12(3)4/h9-10,12-13H,5
InchiKey: FQFAEPRUWZFJGU-MDZDMXLPSA-N
Formula: C15H26O4
SMILES: CCCCC(CC)OC(=O)C=CC(=O)OCC(C)C
Mol. weight [g/mol]: 270.36

Physical Properties

Property code	Value	Unit	Source
gf	-317.08	kJ/mol	Joback Method
hf	-735.87	kJ/mol	Joback Method
hfus	33.34	kJ/mol	Joback Method
hvap	66.48	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.254		Crippen Method
mcvol	232.790	ml/mol	McGowan Method
pc	1602.56	kPa	Joback Method
rinpol	1740.00		NIST Webbook
tb	698.46	K	Joback Method
tc	884.01	K	Joback Method
tf	368.05	K	Joback Method
vc	0.891	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.63	J/mol×K	698.46	Joback Method
cpg	671.72	J/mol×K	729.38	Joback Method
cpg	686.98	J/mol×K	760.31	Joback Method
cpg	701.42	J/mol×K	791.23	Joback Method
cpg	715.06	J/mol×K	822.16	Joback Method
cpg	727.92	J/mol×K	853.08	Joback Method
cpg	740.00	J/mol×K	884.01	Joback Method
dvisc	0.0019655	Pa×s	368.05	Joback Method
dvisc	0.0008087	Pa×s	423.12	Joback Method

dvisc	0.0004083	Pa×s	478.19	Joback Method
dvisc	0.0002374	Pa×s	533.25	Joback Method
dvisc	0.0001528	Pa×s	588.32	Joback Method
dvisc	0.0001060	Pa×s	643.39	Joback Method
dvisc	0.0000779	Pa×s	698.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348679&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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