

Fumaric acid, 2-heptyl isobutyl ester

Inchi:	InChI=1S/C15H26O4/c1-5-6-7-8-13(4)19-15(17)10-9-14(16)18-11-12(2)3/h9-10,12-13H,5
InchiKey:	HSAFRQVMNUQKPW-MDZDMXLPSA-N
Formula:	C15H26O4
SMILES:	CCCCC(C)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	1759.00		NIST Webbook
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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/molxK	698.46	Joback Method
cpg	671.72	J/molxK	729.38	Joback Method
cpg	686.98	J/molxK	760.31	Joback Method
cpg	701.42	J/molxK	791.23	Joback Method
cpg	715.06	J/molxK	822.16	Joback Method
cpg	727.92	J/molxK	853.08	Joback Method
cpg	740.00	J/molxK	884.01	Joback Method
dvisc	0.0019655	Paxs	368.05	Joback Method

dvisc	0.0008087	Paxs	423.12	Joback Method
dvisc	0.0004083	Paxs	478.19	Joback Method
dvisc	0.0002374	Paxs	533.25	Joback Method
dvisc	0.0001528	Paxs	588.32	Joback Method
dvisc	0.0001060	Paxs	643.39	Joback Method
dvisc	0.0000779	Paxs	698.46	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U348622&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

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