

Fumaric acid, cis-hex-3-enyl isobutyl ester

Inchi:	InChI=1S/C14H22O4/c1-4-5-6-7-10-17-13(15)8-9-14(16)18-11-12(2)3/h5-6,8-9,12H,4,7,1
InchiKey:	FUNUUOONRYZMBG-UEPDSTOUSA-N
Formula:	C14H22O4
SMILES:	CCC=CCCOC(=O)C=CC(=O)OCC(C)C
Mol. weight [g/mol]:	254.32

Physical Properties

Property code	Value	Unit	Source
gf	-242.84	kJ/mol	Joback Method
hf	-592.73	kJ/mol	Joback Method
hfus	34.47	kJ/mol	Joback Method
hvap	64.60	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.641		Crippen Method
mvol	214.400	ml/mol	McGowan Method
pc	1798.51	kPa	Joback Method
rinpol	1741.00		NIST Webbook
rinpol	1741.00		NIST Webbook
tb	680.18	K	Joback Method
tc	869.98	K	Joback Method
tf	366.70	K	Joback Method
vc	0.822	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.30	J/molxK	680.18	Joback Method
cpg	645.26	J/molxK	838.34	Joback Method
cpg	633.33	J/molxK	806.71	Joback Method
cpg	620.69	J/molxK	775.08	Joback Method
cpg	607.33	J/molxK	743.45	Joback Method
cpg	593.20	J/molxK	711.81	Joback Method
cpg	656.50	J/molxK	869.98	Joback Method
dvisc	0.0000822	Paxs	680.18	Joback Method

dvisc	0.0001097	Paxs	627.93	Joback Method
dvisc	0.0001541	Paxs	575.69	Joback Method
dvisc	0.0002319	Paxs	523.44	Joback Method
dvisc	0.0003819	Paxs	471.19	Joback Method
dvisc	0.0007124	Paxs	418.95	Joback Method
dvisc	0.0015872	Paxs	366.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348860&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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