

Fumaric acid, dec-4-enyl isobutyl ester

Inchi:	InChI=1S/C18H30O4/c1-4-5-6-7-8-9-10-11-14-21-17(19)12-13-18(20)22-15-16(2)3/h8-9,
InchiKey:	ICXRNQIODIVYQE-AFAJWACHSA-N
Formula:	C18H30O4
SMILES:	CCCCC=CCCCOC(=O)C=CC(=O)OCC(C)C
Mol. weight [g/mol]:	310.43

Physical Properties

Property code	Value	Unit	Source
gf	-209.16	kJ/mol	Joback Method
hf	-675.29	kJ/mol	Joback Method
hfus	44.83	kJ/mol	Joback Method
hvap	73.50	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	4.202		Crippen Method
mvol	270.760	ml/mol	McGowan Method
pc	1330.04	kPa	Joback Method
rinpol	2121.00		NIST Webbook
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tb	771.70	K	Joback Method
tc	959.35	K	Joback Method
tf	411.78	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	801.20	J/molxK	771.70	Joback Method
cpg	875.10	J/molxK	928.08	Joback Method
cpg	861.99	J/molxK	896.80	Joback Method
cpg	848.07	J/molxK	865.53	Joback Method
cpg	833.33	J/molxK	834.25	Joback Method
cpg	817.71	J/molxK	802.98	Joback Method
cpg	887.44	J/molxK	959.35	Joback Method
dvisc	0.0000489	Paxs	771.70	Joback Method

dvisc	0.0000659	Paxs	711.71	Joback Method
dvisc	0.0000939	Paxs	651.73	Joback Method
dvisc	0.0001435	Paxs	591.74	Joback Method
dvisc	0.0002417	Paxs	531.75	Joback Method
dvisc	0.0004645	Paxs	471.77	Joback Method
dvisc	0.0010798	Paxs	411.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348937&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
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

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