Fumaric acid, pent-4-en-2-yl propyl ester

Inchi: InChI=1S/C12H18O4/c1-4-6-10(3)16-12(14)8-7-11(13)15-9-5-2/h4,7-8,10H,1,5-6,9H2,2-3
InchiKey: FFCNSQCGMWSGEA-BQYQJAHWSA-N
Formula: C12H18O4
SMILES: C=CCC(C)OC(=O)C=CC(=O)OCCC
Mol. weight [g/mol]: 226.27

Physical Properties

Property code	Value	Unit	Source
gf	-252.06	kJ/mol	Joback Method
hf	-543.24	kJ/mol	Joback Method
hfus	27.81	kJ/mol	Joback Method
hvap	59.52	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.004		Crippen Method
mcvol	186.220	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
rinpol	1504.00		NIST Webbook
tb	626.94	K	Joback Method
tc	816.65	K	Joback Method
tf	347.48	K	Joback Method
vc	0.711	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.65	J/mol×K	626.94	Joback Method
cpg	535.74	J/mol×K	785.03	Joback Method
cpg	524.64	J/mol×K	753.41	Joback Method
cpg	512.90	J/mol×K	721.79	Joback Method
cpg	500.50	J/mol×K	690.18	Joback Method
cpg	487.42	J/mol×K	658.56	Joback Method
cpg	546.19	J/mol×K	816.65	Joback Method
dvisc	0.0001266	Pa×s	626.94	Joback Method
dvisc	0.0001662	Pa×s	580.36	Joback Method

dvisc	0.0002288	Pa×s	533.79	Joback Method
dvisc	0.0003348	Pa×s	487.21	Joback Method
dvisc	0.0005310	Pa×s	440.63	Joback Method
dvisc	0.0009391	Pa×s	394.06	Joback Method
dvisc	0.0019354	Pa×s	347.48	Joback Method

Sources

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=U348921&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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