Fumaric acid, heptyl 3-oxobut-2-yl ester

Inchi: InChI=1S/C15H24O5/c1-4-5-6-7-8-11-19-14(17)9-10-15(18)20-13(3)12(2)16/h9-10,13H,4
InchiKey: LZRBSRFCMYHGGG-MDZDMXLPSA-N
Formula: C15H24O5
SMILES: CCCCCCCOC(=O)C=CC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 284.35

Physical Properties

Property code	Value	Unit	Source
gf	-443.56	kJ/mol	Joback Method
hf	-843.17	kJ/mol	Joback Method
hfus	38.46	kJ/mol	Joback Method
hvap	73.61	kJ/mol	Joback Method
log10ws	-3.07		Crippen Method
logp	2.577		Crippen Method
mcvol	234.360	ml/mol	McGowan Method
pc	1675.53	kPa	Joback Method
rinpol	1962.00		NIST Webbook
tb	752.77	K	Joback Method
tc	943.28	K	Joback Method
tf	432.98	K	Joback Method
vc	0.903	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.61	J/mol×K	752.77	Joback Method
cpg	739.97	J/mol×K	911.53	Joback Method
cpg	728.73	J/mol×K	879.77	Joback Method
cpg	716.69	J/mol×K	848.02	Joback Method
cpg	703.83	J/mol×K	816.27	Joback Method
cpg	690.14	J/mol×K	784.52	Joback Method
cpg	750.43	J/mol×K	943.28	Joback Method
dvisc	0.0000820	Pa×s	752.77	Joback Method
dvisc	0.0001080	Pa×s	699.47	Joback Method

dvisc	0.0001488	Pa×s	646.17	Joback Method
dvisc	0.0002172	Pa×s	592.88	Joback Method
dvisc	0.0003417	Pa×s	539.58	Joback Method
dvisc	0.0005938	Pa×s	486.28	Joback Method
dvisc	0.0011820	Pa×s	432.98	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=U348821&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