Fumaric acid, isohexyl 3-methylbut-3-enyl ester

Inchi: InChI=1S/C15H24O4/c1-12(2)6-5-10-18-14(16)7-8-15(17)19-11-9-13(3)4/h7-8,12H,3,5-6

InchiKey: HIMJSEYQNBWVFQ-BQYQJAHWSA-N

Formula: C15H24O4

SMILES: C=C(C)CCOC(=O)C=CC(=O)OCCCC(C)C

Mol. weight [g/mol]: 268.35

Physical Properties

Property code	Value	Unit	Source
gf	-235.35	kJ/mol	Joback Method
hf	-614.95	kJ/mol	Joback Method
hfus	34.27	kJ/mol	Joback Method
hvap	66.28	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.031		Crippen Method
mcvol	228.490	ml/mol	McGowan Method
pc	1653.80	kPa	Joback Method
rinpol	1823.00		NIST Webbook
rinpol	1823.00		NIST Webbook
tb	695.46	K	Joback Method
tc	883.01	K	Joback Method
tf	367.33	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	630.92	J/mol×K	695.46	Joback Method
cpg	646.40	J/mol×K	726.72	Joback Method
cpg	661.08	J/mol×K	757.98	Joback Method
cpg	674.96	J/mol×K	789.24	Joback Method
cpg	688.07	J/mol×K	820.49	Joback Method
cpg	700.43	J/mol×K	851.75	Joback Method
cpg	712.06	J/mol×K	883.01	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=U348904&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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