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

Inchi: InChI=1S/C15H24O4/c1-4-5-6-7-11-18-14(16)8-9-15(17)19-12-10-13(2)3/h8-9H,2,4-7,10
InchiKey: QGCBHXMDUINJFD-CMDGGOBGSA-N
Formula: C15H24O4
SMILES: C=C(C)CCOC(=O)C=CC(=O)OCCCCCC
Mol. weight [g/mol]: 268.35

Physical Properties

Property code	Value	Unit	Source
gf	-232.91	kJ/mol	Joback Method
hf	-609.67	kJ/mol	Joback Method
hfus	37.79	kJ/mol	Joback Method
hvap	66.66	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.175		Crippen Method
mcvol	228.490	ml/mol	McGowan Method
pc	1643.09	kPa	Joback Method
rinpol	1865.00		NIST Webbook
tb	695.90	K	Joback Method
tc	880.84	K	Joback Method
tf	382.33	K	Joback Method
vc	0.885	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	630.42	J/mol×K	695.90	Joback Method
cpg	645.67	J/mol×K	726.72	Joback Method
cpg	660.13	J/mol×K	757.55	Joback Method
cpg	673.83	J/mol×K	788.37	Joback Method
cpg	686.80	J/mol×K	819.19	Joback Method
cpg	699.03	J/mol×K	850.02	Joback Method
cpg	710.57	J/mol×K	880.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348905&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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