Fumaric acid, 2-ethylhexyl 3-methylbut-2-en-1-yl ester

Inchi: InChI=1S/C17H28O4/c1-5-7-8-15(6-2)13-21-17(19)10-9-16(18)20-12-11-14(3)4/h9-11,15

InchiKey: OGSWJCBHEPFYDH-MDZDMXLPSA-N

Formula: C17H28O4

SMILES: CCCCC(CC)COC(=O)C=CC(=O)OCC=C(C)C

Mol. weight [g/mol]: 296.40

Physical Properties

Property code	Value	Unit	Source
gf	-226.13	kJ/mol	Joback Method
hf	-664.44	kJ/mol	Joback Method
hfus	40.93	kJ/mol	Joback Method
hvap	71.36	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.812		Crippen Method
mcvol	256.670	ml/mol	McGowan Method
pc	1433.72	kPa	Joback Method
rinpol	2028.00		NIST Webbook
rinpol	2028.00		NIST Webbook
tb	748.70	K	Joback Method
tc	937.95	K	Joback Method
tf	386.55	K	Joback Method
vc	0.991	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.47	J/mol×K	748.70	Joback Method
cpg	759.75	J/mol×K	780.24	Joback Method
cpg	775.16	J/mol×K	811.78	Joback Method
cpg	789.72	J/mol×K	843.33	Joback Method
cpg	803.47	J/mol×K	874.87	Joback Method
cpg	816.42	J/mol×K	906.41	Joback Method
cpg	828.62	J/mol×K	937.95	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405572&Units=SI

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