Fumaric acid, monoamide, N-methallyl-, 2-ethylhexyl ester

Inchi: InChI=1S/C16H27NO3/c1-5-7-8-14(6-2)12-20-16(19)10-9-15(18)17-11-13(3)4/h9-10,14H

InchiKey: DPVRYKFGINGCPJ-MDZDMXLPSA-N

Formula: C16H27NO3

SMILES: C=C(C)CNC(=O)C=CC(=O)OCC(CC)CCCC

Mol. weight [g/mol]: 281.39

Physical Properties

Property code	Value	Unit	Source
gf	-32.54	kJ/mol	Joback Method
hf	-449.90	kJ/mol	Joback Method
hfus	40.77	kJ/mol	Joback Method
hvap	72.53	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	2.994		Crippen Method
mcvol	246.690	ml/mol	McGowan Method
pc	1568.47	kPa	Joback Method
rinpol	2244.00		NIST Webbook
tb	746.09	K	Joback Method
tc	935.65	K	Joback Method
tf	409.03	K	Joback Method
vc	0.953	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	715.79	J/mol×K	746.09	Joback Method
cpg	731.47	J/mol×K	777.68	Joback Method
cpg	746.29	J/mol×K	809.28	Joback Method
cpg	760.28	J/mol×K	840.87	Joback Method
cpg	773.48	J/mol×K	872.46	Joback Method
cpg	785.91	J/mol×K	904.06	Joback Method
cpg	797.63	J/mol×K	935.65	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=U357504&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