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

Inchi: InChI=1S/C14H25NO3/c1-5-7-8-12(6-2)11-18-14(17)10-9-13(16)15(3)4/h9-10,12H,5-8,1

InchiKey: PMOFUGINNHITNZ-MDZDMXLPSA-N

Formula: C14H25NO3

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

Mol. weight [g/mol]: 255.35

Physical Properties

Property code	Value	Unit	Source
gf	-107.28	kJ/mol	Joback Method
hf	-510.20	kJ/mol	Joback Method
hfus	36.10	kJ/mol	Joback Method
hvap	64.27	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	2.390		Crippen Method
mcvol	222.810	ml/mol	McGowan Method
pc	1743.37	kPa	Joback Method
rinpol	2062.00		NIST Webbook
rinpol	2062.00		NIST Webbook
tb	666.04	K	Joback Method
tc	848.98	K	Joback Method
tf	382.02	K	Joback Method
vc	0.842	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.90	J/mol×K	666.04	Joback Method
cpg	627.81	J/mol×K	696.53	Joback Method
cpg	642.90	J/mol×K	727.02	Joback Method
cpg	657.20	J/mol×K	757.51	Joback Method
cpg	670.74	J/mol×K	788.00	Joback Method
cpg	683.54	J/mol×K	818.49	Joback Method
cpg	695.64	J/mol×K	848.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357503&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