

Fumaric acid, 2-ethylhexyl hex-4-yn-3-yl ester

Inchi: InChI=1S/C18H28O4/c1-5-9-11-15(7-3)14-21-17(19)12-13-18(20)22-16(8-4)10-6-2/h12-14
InchiKey: WEHJCDUZBXIJRK-OUKQBFOZSA-N
Formula: C18H28O4
SMILES: CC#CC(CC)OC(=O)C=CC(=O)OCC(CC)CCCC
Mol. weight [g/mol]: 308.41

Physical Properties

Property code	Value	Unit	Source
gf	-89.02	kJ/mol	Joback Method
hf	-525.49	kJ/mol	Joback Method
hfus	44.23	kJ/mol	Joback Method
hvap	75.31	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	3.647		Crippen Method
mvol	266.460	ml/mol	McGowan Method
pc	1450.14	kPa	Joback Method
rinpol	2079.00		NIST Webbook
rinpol	2079.00		NIST Webbook
tb	776.10	K	Joback Method
tc	973.70	K	Joback Method
tf	507.96	K	Joback Method
vc	1.022	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	778.28	J/molxK	776.10	Joback Method
cpg	794.85	J/molxK	809.03	Joback Method
cpg	810.44	J/molxK	841.97	Joback Method
cpg	825.08	J/molxK	874.90	Joback Method
cpg	838.79	J/molxK	907.83	Joback Method
cpg	851.58	J/molxK	940.76	Joback Method
cpg	863.49	J/molxK	973.70	Joback Method

Sources

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=U405573&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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