Fumaric acid, 2-ethylbutyl tridec-2-yn-1-yl ester

Inchi: InChI=1S/C23H38O4/c1-4-7-8-9-10-11-12-13-14-15-16-19-26-22(24)17-18-23(25)27-20-
InchiKey: DYPNBMXUZSLRAP-ISLYRVAYSA-N
Formula: C23H38O4
SMILES: CCCCCCCCCCC#CCOC(=O)C=CC(=O)OCC(CC)CC
Mol. weight [g/mol]: 378.55

Physical Properties

Property code	Value	Unit	Source
gf	-44.48	kJ/mol	Joback Method
hf	-623.41	kJ/mol	Joback Method
hfus	60.70	kJ/mol	Joback Method
hvap	86.83	kJ/mol	Joback Method
log10ws	-6.58		Crippen Method
logp	5.599		Crippen Method
mcvol	336.910	ml/mol	McGowan Method
pc	1031.25	kPa	Joback Method
rinpol	2661.00		NIST Webbook
rinpol	2661.00		NIST Webbook
tb	890.94	K	Joback Method
tc	1092.76	K	Joback Method
tf	579.31	K	Joback Method
vc	1.308	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1076.00	J/mol×K	890.94	Joback Method
cpg	1093.88	J/mol×K	924.58	Joback Method
cpg	1110.60	J/mol×K	958.21	Joback Method
cpg	1126.18	J/mol×K	991.85	Joback Method
cpg	1140.67	J/mol×K	1025.49	Joback Method
cpg	1154.10	J/mol×K	1059.13	Joback Method
cpg	1166.50	J/mol×K	1092.76	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=U405642&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