Fumaric acid, 3-methylbutyl tridec-2-yn-1-yl ester

Inchi: InChI=1S/C22H36O4/c1-4-5-6-7-8-9-10-11-12-13-14-18-25-21(23)15-16-22(24)26-19-17

InchiKey: IRBMCGFOAMSYRC-FOCLMDBBSA-N

Formula: C22H36O4

SMILES: CCCCCCCCCCC#CCOC(=O)C=CC(=O)OCCC(C)C

Mol. weight [g/mol]: 364.52

Physical Properties

Property code	Value	Unit	Source
gf	-52.90	kJ/mol	Joback Method
hf	-602.77	kJ/mol	Joback Method
hfus	58.11	kJ/mol	Joback Method
hvap	84.60	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	5.209		Crippen Method
mcvol	322.820	ml/mol	McGowan Method
pc	1097.90	kPa	Joback Method
rinpol	2566.00		NIST Webbook
tb	868.06	K	Joback Method
tc	1067.08	K	Joback Method
tf	568.04	K	Joback Method
vc	1.252	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1014.79	J/mol×K	868.06	Joback Method
cpg	1032.36	J/mol×K	901.23	Joback Method
cpg	1048.81	J/mol×K	934.40	Joback Method
cpg	1064.19	J/mol×K	967.57	Joback Method
cpg	1078.51	J/mol×K	1000.74	Joback Method
cpg	1091.82	J/mol×K	1033.91	Joback Method
cpg	1104.14	J/mol×K	1067.08	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=U405556&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