4-Ethylbenzoic acid, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C18H24O2/c1-5-7-8-17(13-14(3)4)20-18(19)16-11-9-15(6-2)10-12-16/h9-12,14

InchiKey: ZMVHFIKUBUHYDD-UHFFFAOYSA-N

Formula: C18H24O2

SMILES: CCC#CC(CC(C)C)OC(=O)c1ccc(CC)cc1

Mol. weight [g/mol]: 272.38

Physical Properties

Property code	Value	Unit	Source
gf	167.46	kJ/mol	Joback Method
hf	-172.85	kJ/mol	Joback Method
hfus	34.89	kJ/mol	Joback Method
hvap	69.13	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	4.234		Crippen Method
mcvol	239.560	ml/mol	McGowan Method
pc	1724.59	kPa	Joback Method
rinpol	1965.90		NIST Webbook
tb	727.31	K	Joback Method
tc	944.59	K	Joback Method
tf	479.82	K	Joback Method
vc	0.909	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.97	J/mol×K	727.31	Joback Method
cpg	683.82	J/mol×K	763.52	Joback Method
cpg	700.53	J/mol×K	799.74	Joback Method
cpg	716.13	J/mol×K	835.95	Joback Method
cpg	730.66	J/mol×K	872.16	Joback Method
cpg	744.15	J/mol×K	908.37	Joback Method
cpg	756.64	J/mol×K	944.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292545&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

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

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