4-Ethylbenzoic acid, 2-(1-adamantyl)ethyl ester

Inchi: InChI=1S/C21H28O2/c1-2-15-3-5-19(6-4-15)20(22)23-8-7-21-12-16-9-17(13-21)11-18(10

InchiKey: HJSWANZVUIKIDV-UHFFFAOYSA-N

Formula: C21H28O2

SMILES: CCc1ccc(C(=O)OCCC23CC4CC(CC(C4)C2)C3)cc1

Mol. weight [g/mol]: 312.45

Physical Properties

Property code	Value	Unit	Source
gf	151.75	kJ/mol	Joback Method
hf	-289.37	kJ/mol	Joback Method
hfus	33.66	kJ/mol	Joback Method
hvap	72.89	kJ/mol	Joback Method
log10ws	-5.84		Crippen Method
logp	5.012		Crippen Method
mcvol	257.850	ml/mol	McGowan Method
pc	1672.79	kPa	Joback Method
rinpol	2562.70		NIST Webbook
rinpol	2562.70		NIST Webbook
tb	807.89	K	Joback Method
tc	1037.22	K	Joback Method
tf	507.49	K	Joback Method
vc	0.988	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	840.59	J/mol×K	807.89	Joback Method
cpg	861.99	J/mol×K	846.11	Joback Method
cpg	882.71	J/mol×K	884.33	Joback Method
cpg	902.98	J/mol×K	922.56	Joback Method
cpg	923.04	J/mol×K	960.78	Joback Method
cpg	943.14	J/mol×K	999.00	Joback Method
cpg	963.52	J/mol×K	1037.22	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=U292200&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