4-ethylbenzoic acid, 2-adamantyl ester

Inchi: InChI=1S/C19H24O2/c1-2-12-3-5-15(6-4-12)19(20)21-18-16-8-13-7-14(10-16)11-17(18)9

InchiKey: ZIIYEEGFRAAVLV-UHFFFAOYSA-N

Formula: C19H24O2

SMILES: CCc1ccc(C(=O)OC2C3CC4CC(C3)CC2C4)cc1

Mol. weight [g/mol]: 284.40

Physical Properties

Property code	Value	Unit	Source
hf	-449.85	kJ/mol	Cheméo Relay (1.0)
hfus	35.85	kJ/mol	Joback Method
logp	4.231		Crippen Method
mcvol	229.670	ml/mol	McGowan Method
rinpol	2325.30		NIST Webbook
tb	648.97	K	Cheméo Relay (1.0)
tf	427.17	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.10	J/mol×K	757.22	Joback Method
cpg	751.52	J/mol×K	795.47	Joback Method
cpg	770.54	J/mol×K	833.73	Joback Method
cpg	788.26	J/mol×K	871.98	Joback Method
cpg	804.83	J/mol×K	910.24	Joback Method
cpg	820.35	J/mol×K	948.49	Joback Method
cpg	834.95	J/mol×K	986.75	Joback Method
dvisc	0.0038237	Pa×s	456.81	Joback Method
dvisc	0.0033437	Pa×s	506.88	Joback Method
dvisc	0.0029953	Pa×s	556.95	Joback Method
dvisc	0.0027324	Pa×s	607.01	Joback Method
dvisc	0.0025277	Pa×s	657.08	Joback Method
dvisc	0.0023642	Pa×s	707.15	Joback Method
dvisc	0.0022310	Pa×s	757.22	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292198&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point