4-ethylbenzoic acid, 1-adamantylmethyl ester

Inchi: InChI=1S/C20H26O2/c1-2-14-3-5-18(6-4-14)19(21)22-13-20-10-15-7-16(11-20)9-17(8-15
InchiKey: FLVOKNUCTFWOKW-UHFFFAOYSA-N
Formula: C20H26O2
SMILES: CCc1ccc(C(=O)OCC23CC4CC(CC(C4)C2)C3)cc1
Mol. weight [g/mol]: 298.43

Physical Properties

Property code	Value	Unit	Source
hf	-467.85	kJ/mol	Cheméo Relay (1.0)
hfus	31.07	kJ/mol	Joback Method
logp	4.622		Crippen Method
mcvol	243.760	ml/mol	McGowan Method
rinpol	2443.40		NIST Webbook
rinpol	2443.40		NIST Webbook
tb	663.79	K	Cheméo Relay (1.0)
tf	420.11	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	781.45	J/mol×K	785.01	Joback Method
cpg	802.52	J/mol×K	823.83	Joback Method
cpg	822.82	J/mol×K	862.65	Joback Method
cpg	842.60	J/mol×K	901.47	Joback Method
cpg	862.09	J/mol×K	940.29	Joback Method
cpg	881.54	J/mol×K	979.11	Joback Method
cpg	901.21	J/mol×K	1017.93	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292199&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

Legend

cpg:	Ideal gas heat capacity
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