Phenanthrene, 1,3-difluoro

Inchi: InChI=1S/C14H8F2/c15-10-7-13-11-4-2-1-3-9(11)5-6-12(13)14(16)8-10/h1-8H
InchiKey: CWQMLMUMNMOJFB-UHFFFAOYSA-N
Formula: C14H8F2
SMILES: Fc1cc(F)c2ccc3ccccc3c2c1
Mol. weight [g/mol]: 214.21

Physical Properties

Property code	Value	Unit	Source
gf	-25.80	kJ/mol	Joback Method
hf	-140.25	kJ/mol	Joback Method
hfus	25.09	kJ/mol	Joback Method
hvap	52.67	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	4.271		Crippen Method
mcvol	148.980	ml/mol	McGowan Method
pc	2841.41	kPa	Joback Method
rinpol	1687.00		NIST Webbook
rinpol	1687.00		NIST Webbook
rinpol	290.35		NIST Webbook
rinpol	1686.00		NIST Webbook
rinpol	290.06		NIST Webbook
rinpol	290.35		NIST Webbook
ripol	283.25		NIST Webbook
ripol	283.25		NIST Webbook
tb	597.84	K	Joback Method
tc	828.74	K	Joback Method
tf	378.10	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.97	J/mol×K	597.84	Joback Method
cpg	361.80	J/mol×K	636.32	Joback Method

cpg	373.62	J/mol×K	674.81	Joback Method
cpg	384.52	J/mol×K	713.29	Joback Method
cpg	394.61	J/mol×K	751.77	Joback Method
cpg	403.98	J/mol×K	790.25	Joback Method
cpg	412.72	J/mol×K	828.74	Joback Method

Sources

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=R76103&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume