Phenanthrene, 3,6-difluoro

Inchi: InChI=1S/C14H8F2/c15-11-5-3-9-1-2-10-4-6-12(16)8-14(10)13(9)7-11/h1-8H
InchiKey: YYXWAONYDSGVOU-UHFFFAOYSA-N
Formula: C14H8F2
SMILES: Fc1ccc2ccc3ccc(F)cc3c2c1
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	294.34		NIST Webbook
rinpol	1711.00		NIST Webbook
rinpol	298.87		NIST Webbook
rinpol	1737.00		NIST Webbook
ripol	294.92		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:	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=R76153&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume