

1,1-DIFLUORO-2,5-DIPHENYL-CYCLOPROPABENZENE

Other names:	1,1-Difluoro-2,5-diphenyl-cyclopropabenzene
Inchi:	InChI=1S/C19H12F2/c20-19(21)17-15(13-7-3-1-4-8-13)11-12-16(18(17)19)14-9-5-2-6-10
InchiKey:	OWEGRVCQGPMFPP-UHFFFAOYSA-N
Formula:	C19H12F2
SMILES:	FC1(F)c2c(-c3ccccc3)ccc(-c3ccccc3)c21
Mol. weight [g/mol]:	278.30

Physical Properties

Property code	Value	Unit	Source
af	0.5105		Cheméo Relay (1.0)
gf	107.28	kJ/mol	Joback Method
hf	-100.84	kJ/mol	Cheméo Relay (1.0)
hfus	28.12	kJ/mol	Joback Method
hvap	100.14	kJ/mol	Cheméo Relay (1.0)
ie	8.20	eV	NIST Webbook
log10ws	-6.69		Cheméo Relay (1.0)
logp	5.474		Crippen Method
mcvol	199.970	ml/mol	McGowan Method
pc	2358.78	kPa	Joback Method
tb	651.32	K	Cheméo Relay (1.0)
tc	930.91	K	Cheméo Relay (1.0)
tf	380.62	K	Cheméo Relay (1.0)
vc	0.769	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	536.89	J/mol×K	726.08	Joback Method
cpg	552.21	J/mol×K	767.96	Joback Method
cpg	566.82	J/mol×K	809.85	Joback Method
cpg	581.03	J/mol×K	851.73	Joback Method
cpg	595.13	J/mol×K	893.62	Joback Method
cpg	609.42	J/mol×K	935.50	Joback Method
cpg	624.21	J/mol×K	977.39	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C52326848&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

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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