Alpha,alpha'-diacetyl-4,4'-difluoro-glutaranilide

Inchi: InChI=1S/C21H20F2N2O4/c1-12(26)18(20(28)24-16-7-3-14(22)4-8-16)11-19(13(2)27)21
InchiKey: NGEIWFJRFMSXKY-UHFFFAOYSA-N
Formula: C21H20F2N2O4
SMILES: CC(=O)C(CC(C(C)=O)C(=O)Nc1ccc(F)cc1)C(=O)Nc1ccc(F)cc1
Mol. weight [g/mol]: 402.39
CAS: 807-75-0

Physical Properties

Property code	Value	Unit	Source
gf	-399.90	kJ/mol	Joback Method
hf	-772.81	kJ/mol	Joback Method
hfus	53.16	kJ/mol	Joback Method
hvap	105.66	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.342		Crippen Method
mcvol	289.010	ml/mol	McGowan Method
pc	1739.01	kPa	Joback Method
tb	1056.68	K	Joback Method
tc	1297.12	K	Joback Method
tf	680.53	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	919.62	J/mol×K	1056.68	Joback Method
cpg	928.75	J/mol×K	1096.75	Joback Method
cpg	936.81	J/mol×K	1136.83	Joback Method
cpg	943.87	J/mol×K	1176.90	Joback Method
cpg	950.05	J/mol×K	1216.97	Joback Method
cpg	955.42	J/mol×K	1257.05	Joback Method
cpg	960.07	J/mol×K	1297.12	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=C807750&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume