Isophthalic acid, 1-adamantylmethyl ethyl ester

Inchi: InChI=1S/C21H26O4/c1-2-24-19(22)17-4-3-5-18(9-17)20(23)25-13-21-10-14-6-15(11-21

InchiKey: HPTPOGNGLYNXJS-UHFFFAOYSA-N

Formula: C21H26O4

SMILES: CCOC(=O)c1cccc(C(=O)OCC23CC4CC(CC(C4)C2)C3)c1

Mol. weight [g/mol]: 342.43

Physical Properties

Property code	Value	Unit	Source
gf	-82.17	kJ/mol	Joback Method
hf	-534.17	kJ/mol	Joback Method
hfus	36.45	kJ/mol	Joback Method
hvap	82.04	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	4.237		Crippen Method
mcvol	265.290	ml/mol	McGowan Method
pc	1737.56	kPa	Joback Method
rinpol	2802.00		NIST Webbook
tb	884.18	K	Joback Method
tc	1116.97	K	Joback Method
tf	579.65	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	892.11	J/mol×K	884.18	Joback Method
cpg	912.18	J/mol×K	922.98	Joback Method
cpg	931.89	J/mol×K	961.78	Joback Method
cpg	951.48	J/mol×K	1000.57	Joback Method
cpg	971.18	J/mol×K	1039.37	Joback Method
cpg	991.20	J/mol×K	1078.17	Joback Method
cpg	1011.79	J/mol×K	1116.97	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=U343960&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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