

Agglomerone

Inchi:	InChI=1S/C13H18O4/c1-7(2)11(15)10-8(14)6-9(17-5)13(3,4)12(10)16/h6-7,10H,1-5H3
InchiKey:	NQBCCNHGJDEUDS-UHFFFAOYSA-N
Formula:	C13H18O4
SMILES:	<chem>COC1=CC(=O)C(C(=O)C(C)C)C(=O)C1(C)C</chem>
Mol. weight [g/mol]:	238.28

Physical Properties

Property code	Value	Unit	Source
gf	-391.38	kJ/mol	Joback Method
hf	-741.60	kJ/mol	Joback Method
hfus	15.15	kJ/mol	Joback Method
hvap	61.72	kJ/mol	Joback Method
log10ws	-1.71		Crippen Method
logp	1.536		Crippen Method
mcvol	189.450	ml/mol	McGowan Method
pc	2258.96	kPa	Joback Method
ripol	1669.00		NIST Webbook
ripol	1669.00		NIST Webbook
ripol	2356.00		NIST Webbook
ripol	2381.00		NIST Webbook
ripol	2381.00		NIST Webbook
ripol	2381.00		NIST Webbook
ripol	2356.00		NIST Webbook
ripol	2381.00		NIST Webbook
tb	727.59	K	Joback Method
tc	961.49	K	Joback Method
tf	470.19	K	Joback Method
vc	0.712	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.21	J/molxK	727.59	Joback Method
cpg	571.08	J/molxK	766.57	Joback Method

cpg	588.07	J/mol×K	805.56	Joback Method
cpg	604.23	J/mol×K	844.54	Joback Method
cpg	619.57	J/mol×K	883.52	Joback Method
cpg	634.16	J/mol×K	922.51	Joback Method
cpg	648.02	J/mol×K	961.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R323374&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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