

5A-Pregnanolone arachidonate

Inchi:	InChI=1S/C41H64O3/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-39(43)44-3
InchiKey:	UOBMZBMPGJNZCK-IOKQDMLZSA-N
Formula:	C41H64O3
SMILES:	CCCCC=CCC=CCC=CCC=CCCC(=O)OC1CCC2(C)C(CCC3C2CCC2(C)C(C(C)=O)O
Mol. weight [g/mol]:	604.95

Physical Properties

Property code	Value	Unit	Source
gf	393.06	kJ/mol	Joback Method
hf	-568.55	kJ/mol	Joback Method
hfus	80.87	kJ/mol	Joback Method
hvap	119.57	kJ/mol	Joback Method
log10ws	-12.54		Crippen Method
logp	11.292		Crippen Method
mcvol	536.920	ml/mol	McGowan Method
pc	557.83	kPa	Joback Method
rinpola	4750.00		NIST Webbook
rinpola	4750.00		NIST Webbook
tb	1314.39	K	Joback Method
tc	1643.45	K	Joback Method
tf	738.60	K	Joback Method
vc	2.062	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2371.76	J/molxK	1314.39	Joback Method
cpg	2460.56	J/molxK	1369.23	Joback Method
cpg	2558.71	J/molxK	1424.08	Joback Method
cpg	2667.52	J/molxK	1478.92	Joback Method
cpg	2788.30	J/molxK	1533.76	Joback Method
cpg	2922.36	J/molxK	1588.60	Joback Method
cpg	3071.01	J/molxK	1643.45	Joback Method

Sources

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=R164100&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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

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