Ramelteon

Other names: Rozerem
(S)-N-[2-(1,6,7,8-tetrahydro-2H-indeno-[5,4-b]furan-8-yl)ethyl]propionamide
Inchi: InChI=1S/C16H21NO2/c1-2-15(18)17-9-7-12-4-3-11-5-6-14-13(16(11)12)8-10-19-14/h5-
InchiKey: YLXDSYKOBKBWJQ-UHFFFAOYSA-N
Formula: C16H21NO2
SMILES: CCC(=O)NCCC1CCc2ccc3c(c21)CCO3
Mol. weight [g/mol]: 259.34
CAS: 196597-26-9

Physical Properties

Property code	Value	Unit	Source
gf	170.92	kJ/mol	Joback Method
hf	-196.62	kJ/mol	Joback Method
hfus	39.95	kJ/mol	Joback Method
hvap	73.30	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	2.568		Crippen Method
mcvol	208.240	ml/mol	McGowan Method
pc	2250.40	kPa	Joback Method
rinpol	2417.00		NIST Webbook
rinpol	2417.00		NIST Webbook
tb	756.24	K	Joback Method
tc	977.95	K	Joback Method
tf	503.34	K	Joback Method
vc	0.800	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.05	J/mol×K	756.24	Joback Method
cpg	641.86	J/mol×K	793.19	Joback Method
cpg	656.70	J/mol×K	830.14	Joback Method
cpg	670.67	J/mol×K	867.09	Joback Method
cpg	683.88	J/mol×K	904.05	Joback Method

cpg	696.44	J/mol×K	941.00	Joback Method
cpg	708.44	J/mol×K	977.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C196597269&Units=SI
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

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