(E)-(1R,2S,4R)-1,7,7-Trimethylbicyclo[2.2.1]heptan-2-yl 3-(benzo[d][1,3]dioxol-5-yl)acrylate

InChI: InChI=1S/C20H24O4/c1-19(2)14-8-9-20(19,3)17(11-14)24-18(21)7-5-13-4-6-15-16(10-13)23-12-22-15/h4-7,10,14,17H,8-9,11-12H2,1-3H3/b7-5+/t14-,17+,20+/m1/s1

InChIKey: PYUDOHXLMHGZJD-FNORWQNLSA-N

Formula: C20H24O4

SMILES: CC1(C)C2CCC1(C)C(OC(=O)C=Cc1ccc3c(c1)OCO3)C2

Mol. weight [g/mol]: 328.40

CAS: 400771-30-4

Physical Properties

Property code	Value	Unit	Source
gf	36.19	kJ/mol	Joback Method
hf	-411.74	kJ/mol	Joback Method
hfus	40.55	kJ/mol	Joback Method
hvap	79.15	kJ/mol	Joback Method
log10ws	-5.15		Crippen Method
logp	4.187		Crippen Method
mcvol	251.200	ml/mol	McGowan Method
pc	1915.26	kPa	Joback Method
rinpol	2652.90		NIST Webbook
rinpol	2652.90		NIST Webbook
tb	848.29	K	Joback Method
tc	1091.85	K	Joback Method
tf	580.70	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	818.92	J/mol×K	848.29	Joback Method
cpg	840.83	J/mol×K	888.88	Joback Method
cpg	863.30	J/mol×K	929.48	Joback Method
cpg	886.72	J/mol×K	970.07	Joback Method
cpg	911.49	J/mol×K	1010.67	Joback Method
cpg	938.03	J/mol×K	1051.26	Joback Method
cpg	966.73	J/mol×K	1091.85	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=C400771304&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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