(Z)-«gamma»-Curcumen-12-yl 2-methylbutyrate

Inchi: InChI=1S/C20H32O2/c1-6-17(4)20(21)22-14-16(3)8-7-9-18(5)19-12-10-15(2)11-13-19/h8
InchiKey: RASDHGWJDPAGMV-XYODZVPOSA-N
Formula: C20H32O2
SMILES: CCC(C)C(=O)OCC(C)=CCCC(C)C1=CC=C(C)CC1
Mol. weight [g/mol]: 304.47

Physical Properties

Property code	Value	Unit	Source
gf	23.21	kJ/mol	Joback Method
hf	-436.78	kJ/mol	Joback Method
hfus	34.62	kJ/mol	Joback Method
hvap	71.18	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	5.605		Crippen Method
mcvol	276.340	ml/mol	McGowan Method
pc	1332.96	kPa	Joback Method
rinpol	2025.00		NIST Webbook
rinpol	2025.00		NIST Webbook
tb	768.95	K	Joback Method
tc	971.56	K	Joback Method
tf	376.46	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	828.63	J/mol×K	768.95	Joback Method
cpg	847.83	J/mol×K	802.72	Joback Method
cpg	865.89	J/mol×K	836.49	Joback Method
cpg	882.85	J/mol×K	870.25	Joback Method
cpg	898.75	J/mol×K	904.02	Joback Method
cpg	913.65	J/mol×K	937.79	Joback Method
cpg	927.59	J/mol×K	971.56	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R233266&Units=SI

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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