2-methyl-2-butenyl-d-3 octanoate

Inchi: InChI=1S/C13H24O2/c1-4-6-7-8-9-10-13(14)15-11-12(3)5-2/h5H,4,6-11H2,1-3H3/b12-5+
InchiKey: IMJCKKFLXZPADU-QNCRELPCSA-N
Formula: C13H21D3O2
SMILES: CC=C(C)COC(=O)CCCCCCC
Mol. weight [g/mol]: 215.35

Physical Properties

Property code	Value	Unit	Source
gf	-103.67	kJ/mol	Joback Method
hf	-449.02	kJ/mol	Joback Method
hfus	31.10	kJ/mol	Joback Method
hvap	53.73	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.856		Crippen Method
mcvol	197.170	ml/mol	McGowan Method
pc	1790.91	kPa	Joback Method
ripol	1767.00		NIST Webbook
ripol	1767.00		NIST Webbook
tb	577.17	K	Joback Method
tc	754.87	K	Joback Method
tf	289.39	K	Joback Method
vc	0.768	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.58	J/mol×K	577.17	Joback Method
cpg	511.74	J/mol×K	606.79	Joback Method
cpg	527.18	J/mol×K	636.40	Joback Method
cpg	541.94	J/mol×K	666.02	Joback Method
cpg	556.03	J/mol×K	695.64	Joback Method
cpg	569.46	J/mol×K	725.25	Joback Method
cpg	582.27	J/mol×K	754.87	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=R322475&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume