5-((E)-2-Methylbut-2-enamido)pentyl (E)-2-methylbut-2-enoate

Inchi: InChI=1S/C15H25NO3/c1-5-12(3)14(17)16-10-8-7-9-11-19-15(18)13(4)6-2/h5-6H,7-11H2

InchiKey: JDACUBWIUVRIHV-BYDSPXIWSA-N

Formula: C15H25NO3

SMILES: CC=C(C)C(=O)NCCCCCOC(=O)C(C)=CC

Mol. weight [g/mol]: 267.36

Physical Properties

Property code	Value	Unit	Source
gf	-54.69	kJ/mol	Joback Method
hf	-441.98	kJ/mol	Joback Method
hfus	41.88	kJ/mol	Joback Method
hvap	71.40	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	2.748		Crippen Method
mcvol	232.600	ml/mol	McGowan Method
pc	1704.71	kPa	Joback Method
rinpol	2200.00		NIST Webbook
rinpol	2200.00		NIST Webbook
tb	731.01	K	Joback Method
tc	923.96	K	Joback Method
tf	395.48	K	Joback Method
vc	0.902	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	660.10	J/mol×K	731.01	Joback Method
cpg	675.36	J/mol×K	763.17	Joback Method
cpg	689.78	J/mol×K	795.33	Joback Method
cpg	703.43	J/mol×K	827.48	Joback Method
cpg	716.32	J/mol×K	859.64	Joback Method
cpg	728.52	J/mol×K	891.80	Joback Method
cpg	740.05	J/mol×K	923.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373715&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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