But-2-enamide, N,N-dioctyl-3-methyl-

Inchi: InChI=1S/C21H41NO/c1-5-7-9-11-13-15-17-22(21(23)19-20(3)4)18-16-14-12-10-8-6-2/h1
InchiKey: UTDLCLJMCKSDLU-UHFFFAOYSA-N
Formula: C21H41NO
SMILES: CCCCCCCCN(CCCCCCCC)C(=O)C=C(C)C
Mol. weight [g/mol]: 323.56

Physical Properties

Property code	Value	Unit	Source
gf	179.47	kJ/mol	Joback Method
hf	-414.39	kJ/mol	Joback Method
hfus	53.66	kJ/mol	Joback Method
hvap	71.17	kJ/mol	Joback Method
log10ws	-6.81		Crippen Method
logp	6.502		Crippen Method
mcvol	314.000	ml/mol	McGowan Method
pc	1029.92	kPa	Joback Method
rinpol	2298.00		NIST Webbook
rinpol	2298.00		NIST Webbook
tb	750.23	K	Joback Method
tc	926.12	K	Joback Method
tf	389.79	K	Joback Method
vc	1.216	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	955.72	J/mol×K	750.23	Joback Method
cpg	975.75	J/mol×K	779.54	Joback Method
cpg	994.82	J/mol×K	808.86	Joback Method
cpg	1012.98	J/mol×K	838.17	Joback Method
cpg	1030.27	J/mol×K	867.49	Joback Method
cpg	1046.74	J/mol×K	896.80	Joback Method
cpg	1062.45	J/mol×K	926.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308242&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