Fumaric acid, monoamide, N-(4-chlorophenyl)-, neopentyl ester

Inchi: InChI=1S/C15H18ClNO3/c1-15(2,3)10-20-14(19)9-8-13(18)17-12-6-4-11(16)5-7-12/h4-9H

InchiKey: BMLAGWCMYYTMAV-CMDGGOBGSA-N

Formula: C15H18ClNO3

SMILES: CC(C)(C)COC(=O)C=CC(=O)Nc1ccc(Cl)cc1

Mol. weight [g/mol]: 295.76

Physical Properties

Property code	Value	Unit	Source
gf	-24.12	kJ/mol	Joback Method
hf	-339.05	kJ/mol	Joback Method
hfus	34.73	kJ/mol	Joback Method
hvap	77.31	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.424		Crippen Method
mcvol	225.380	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
rinpol	2538.00		NIST Webbook
tb	792.95	K	Joback Method
tc	1017.99	K	Joback Method
tf	499.76	K	Joback Method
vc	0.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.28	J/mol×K	792.95	Joback Method
cpg	636.35	J/mol×K	830.46	Joback Method
cpg	648.43	J/mol×K	867.96	Joback Method
cpg	659.60	J/mol×K	905.47	Joback Method
cpg	669.94	J/mol×K	942.98	Joback Method
cpg	679.51	J/mol×K	980.48	Joback Method
cpg	688.39	J/mol×K	1017.99	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=U357516&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